Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptau129pxo

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

```
 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  JAN 02  STN pricing information for 2008 now available
 NEWS  3  JAN 16  CAS patent coverage enhanced to include exemplified
                  prophetic substances
 NEWS  4  JAN 28  USPATFULL, USPAT2, and USPATOLD enhanced with new
                  custom IPC display formats
 NEWS  5  JAN 28  MARPAT searching enhanced
 NEWS  6  JAN 28  USGENE now provides USPTO sequence data within 3 days
                  of publication
 NEWS  7  JAN 28  TOXCENTER enhanced with reloaded MEDLINE segment
 NEWS  8  JAN 28  MEDLINE and LMEDLINE reloaded with enhancements
 NEWS  9  FEB 08  STN Express, Version 8.3, now available
 NEWS 10  FEB 20  PCI now available as a replacement to DPCI
 NEWS 11  FEB 25  IFIREF reloaded with enhancements
 NEWS 12  FEB 25  IMSPRODUCT reloaded with enhancements
 NEWS 13  FEB 29  WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                  U.S. National Patent Classification
 NEWS 14  MAR 31  IFICDB, IFIPAT, and IFIUDB enhanced with new custom
                  IPC display formats
 NEWS 15  MAR 31  CAS REGISTRY enhanced with additional experimental
                  spectra
 NEWS 16  MAR 31  CA/CAplus and CASREACT patent number format for U.S.
                  applications updated
 NEWS 17  MAR 31  LPCI now available as a replacement to LDPCI
 NEWS 18  MAR 31  EMBASE, EMBAL, and LEMBASE reloaded with enhancements
 NEWS 19  APR 04  STN AnaVist, Version 1, to be discontinued
 NEWS 20  APR 15  WPIDS, WPINDEX, and WPIX enhanced with new
                  predefined hit display formats
 NEWS 21  APR 28  EMBASE Controlled Term thesaurus enhanced
 NEWS 22  APR 28  IMSRESEARCH reloaded with enhancements
 NEWS 23  MAY 30  INPAFAMDB now available on STN for patent family
                  searching
 NEWS 24  MAY 30  DGENE, PCTGEN, and USGENE enhanced with new homology
                  sequence search option
 NEWS 25  JUN 06  EPFULL enhanced with 260,000 English abstracts
 NEWS 26  JUN 06  KOREAPAT updated with 41,000 documents

 NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8
```

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:49:38 ON 09 JUN 2008

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:49:47 ON 09 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 JUN 2008 HIGHEST RN 1026208-38-7
DICTIONARY FILE UPDATES: 6 JUN 2008 HIGHEST RN 1026208-38-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

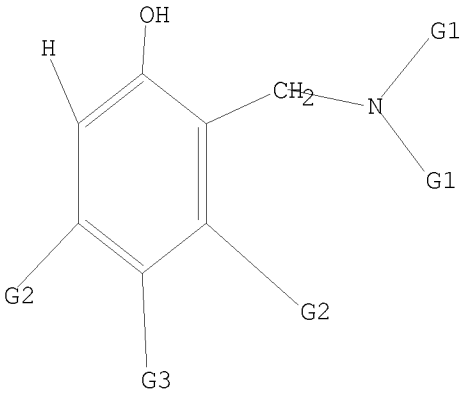
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10511661.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G2 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3 H,Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,CF3,CCl3,Cl,Br,F,I

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 14:54:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      653 TO ITERATE

100.0% PROCESSED      653 ITERATIONS                                4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        11527 TO    14593
PROJECTED ANSWERS:               4 TO      200

L2            4 SEA SSS SAM L1

=> search l1
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:54:13 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    12686 TO ITERATE

100.0% PROCESSED    12686 ITERATIONS                               72 ANSWERS
SEARCH TIME: 00.00.01

L3           72 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     181.58     181.79

FILE 'CAPLUS' ENTERED AT 14:54:18 ON 09 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
```

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN. Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 9 Jun 2008 VOL 148 ISS 24
FILE LAST UPDATED: 8 Jun 2008 (20080608/ED)

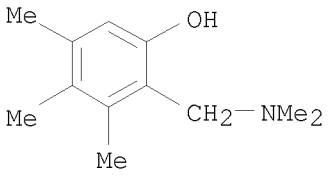
Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l3
L4 37 L3

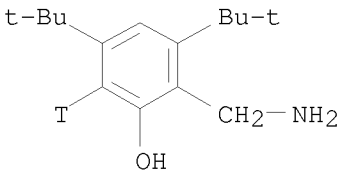
=> d l4 fbib ab hitstr 1-37

L4 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:440649 CAPLUS
DN 148:402897
TI Long chain phenols. Part 42a. Phenolic structure and color in Mannich reaction products
AU Tyman, John H. P.; Patel, Mahesh
CS Department of Chemistry, Brunel University, Uxbridge, Middlesex, UB8 3PH, UK
SO Journal of Chemical Research (2007), (1), 34-37
CODEN: JCROA4
PB Science Reviews
DT Journal
LA English
AB Mannich reactions were carried out with a variety of model alkylphenols and Me2NH, MeNH2, and HN[(CH2)2NH2]2 to trace the origin of persistent colored products occurring in related reactions with pentadeca(e)nylphenol and 4-tert-alkylphenols. It was found to be attributable to the presence of resorcinolic impurities.
IT 89240-10-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(phenolic structure and color in Mannich reaction products)
RN 89240-10-8 CAPLUS
CN Phenol, 2-[(dimethylamino)methyl]-3,4,5-trimethyl- (CA INDEX NAME)



RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:859383 CAPLUS
DN 142:373475
TI Transition metal catalyzed sodium borotritide reductions: a useful alternative to the use of tritium gas
AU Tang, Yui S.; Liu, Wensheng; Chaudhary, Ashok; Melillo, David G.; Dean, Dennis C.
CS Merck Research Laboratories, Rahway, NJ, 07065, USA
SO Synthesis and Applications of Isotopically Labelled Compounds, Proceedings of the International Symposium, 8th, Boston, MA, United States, June 1-5, 2003 (2004), Meeting Date 2003, 71-74. Editor(s): Dean, Dennis C.; Filer, Crist N.; McCarthy, Keith E. Publisher: John Wiley & Sons Ltd., Chichester, UK.
CODEN: 69FZAZ; ISBN: 0-470-86365-X
DT Conference
LA English
OS CASREACT 142:373475
AB Sodium borotritide can be used in combination with transition metal additives for reduction of aryl halides and olefins as an alternative to traditional catalytic tritium gas reduction This methodol. produces high specific activity product, demonstrates excellent chemoselectivity, and eliminates undesired tritium exchange.
IT 849367-52-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(chemoselective preparation of tritium labeled arenes via reductive dehalogenation of arylhalides with sodium borotritide and palladium acetate)
RN 849367-52-8 CAPLUS
CN Phen-2-t-ol, 6-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:2832 CAPLUS
DN 140:59400
TI Preparation of aminoalkylphenols as antimalarials active against drug-resistant Plasmodia.
IN Dorn, Conrad P.; Powles, Mary Ann; Walsh, Thomas F.; Wyvratt, Matthew J.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	WO 2004000783	A1	20031231	WO 2003-US19393		20030620
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
				US 2002-391361P	P	20020624
	CA 2490243	A1	20031231	CA 2003-2490243		20030620
				US 2002-391361P	P	20020624
				WO 2003-US19393	W	20030620
	AU 2003251574	A1	20040106	AU 2003-251574		20030620
				US 2002-391361P	P	20020624
				WO 2003-US19393	W	20030620
	EP 1517879	A1	20050330	EP 2003-761147		20030620
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
				US 2002-391361P	P	20020624
				WO 2003-US19393	W	20030620
	JP 2005534676	T	20051117	JP 2004-515965		20030620
				US 2002-391361P	P	20020624
				WO 2003-US19393	W	20030620
	US 20050234265	A1	20051020	US 2004-511661		20041018
				US 2002-391361P	P	20020624
				WO 2003-US19393	W	20030620

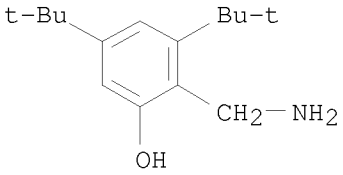
OS MARPAT 140:59400

AB Title compds. [I; R5, R1a, R1 = H, alkyl, halo, alkoxy, cycloalkyl, aryl, trihalovinyl, said aryl optionally substituted with 1-3 Ra; R2 = H, alkyl, C3-10 cycloalkyl; taken together with any intervening atoms can form a 3-7 membered carbocyclyl, heterocyclyl unsatd., said heterocyclic ring containing 1-2 O, CO, S, SO, SO2, N, NR2a and optionally substituted by 1-3 Ra; R2a = H , alkyl; R3, R3a = H , halo, alkyl, C3-10 cycloalkyl, aryl, said aryl and alkyl optionally substituted with 1-3 Ra; R3R3a = atoms to form a 3-7 membered carbocyclyl, heterocyclyl saturated or unsatd., said heterocyclic ring containing 1-2 O, CO, S, SO, SO2, N, NR2a and optionally substituted by 1-3 Ra; R4 = H, halo, alkyl, trihaloalkyl; Ra = alkoxy, alkyl, CF3, NO2, amino, cyano, alkylamino, halo; n = 1-3], were prepared Thus, 3-tert-butylphenol and N-hydroxymethyl-2-chloroacetamide were added in portions to a vigorously stirred solution of AcOH and H2SO4 at 0°; the reaction mixture was allowed to warm to room temperature over several hours, and stirring was maintained for a total of 20 h to give a product which was heated in aqueous HCl at 85° for 3 h to give 2-aminomethyl-5-tert-butylphenol hydrochloride. I inhibited Plasmodium falciparum with IC50<1 μg/mL.

IT 51571-04-1P 84210-35-5P 639069-27-5P
639069-29-7P 639069-31-1P 639069-33-3P
639069-34-4P 639069-35-5P 639069-36-6P
639069-37-7P 639069-38-8P 639069-39-9P
639069-40-2P 639069-41-3P 639069-42-4P
639069-49-1P 639069-58-2P 639069-59-3P
639069-60-6P 639069-62-8P 639069-64-0P

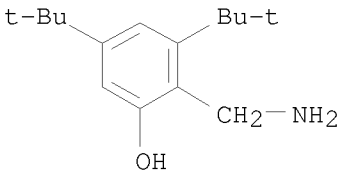
639069-73-1P 639069-76-4P 639069-77-5P
639069-78-6P 639069-79-7P 639069-80-0P
639069-83-3P 639069-88-8P 639069-90-2P
639069-92-4P 639070-01-2P 639070-04-5P
639070-05-6P 639070-06-7P 639070-08-9P
639070-64-7P 639070-65-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminoalkylphenols as antimalarials active against drug-resistant Plasmodia)

RN 51571-04-1 CAPLUS
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

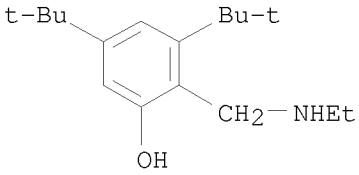


● HCl

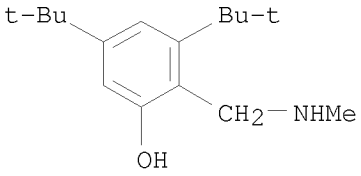
RN 84210-35-5 CAPLUS
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



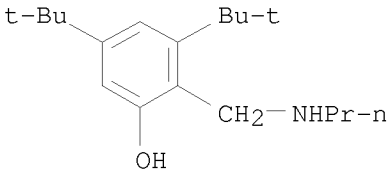
RN 639069-27-5 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(ethylamino)methyl]- (CA INDEX NAME)



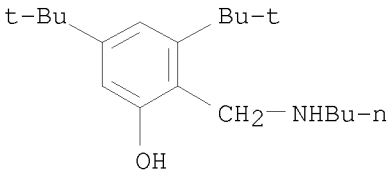
RN 639069-29-7 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(methylamino)methyl]- (CA INDEX NAME)



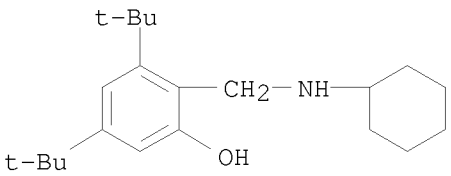
RN 639069-31-1 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(propylamino)methyl]- (CA INDEX NAME)



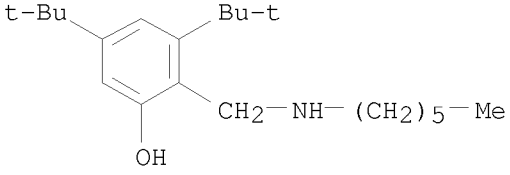
RN 639069-33-3 CAPLUS
CN Phenol, 2-[(butylamino)methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



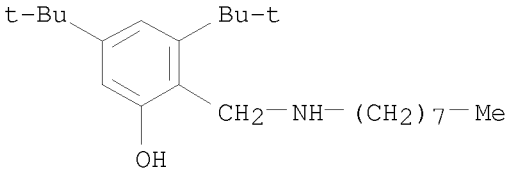
RN 639069-34-4 CAPLUS
CN Phenol, 2-[(cyclohexylamino)methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



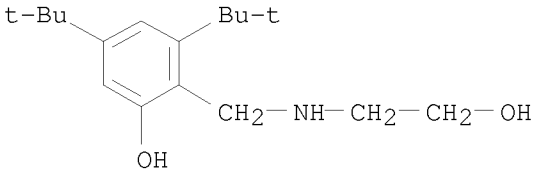
RN 639069-35-5 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(hexylamino)methyl]- (CA INDEX NAME)



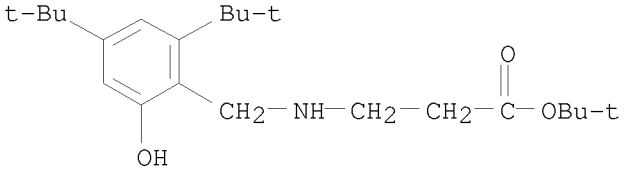
RN 639069-36-6 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(octylamino)methyl]- (CA INDEX NAME)



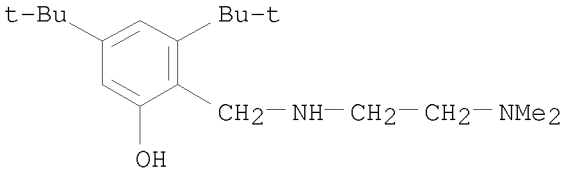
RN 639069-37-7 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(2-hydroxyethyl)amino]methyl]- (CA INDEX NAME)



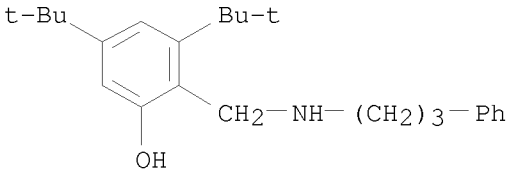
RN 639069-38-8 CAPLUS
CN β-Alanine, N-[[2,4-bis(1,1-dimethylethyl)-6-hydroxyphenyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



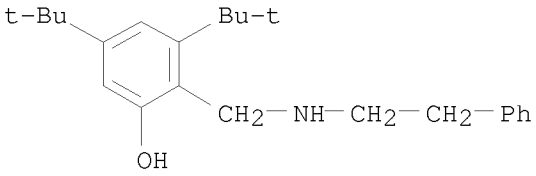
RN 639069-39-9 CAPLUS
CN Phenol, 2-[[[2-(dimethylamino)ethyl]amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



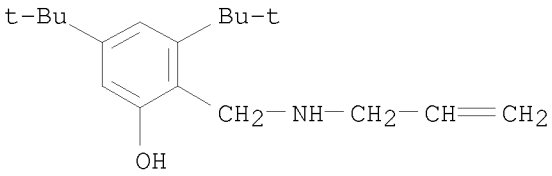
RN 639069-40-2 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(3-phenylpropyl)amino]methyl]- (CA INDEX NAME)



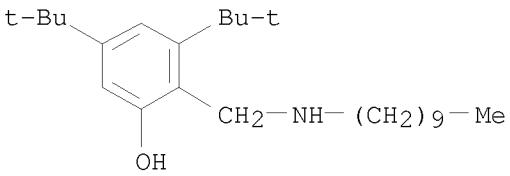
RN 639069-41-3 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(2-phenylethyl)amino]methyl]- (CA INDEX NAME)



RN 639069-42-4 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(2-propen-1-ylamino)methyl]- (CA INDEX NAME)

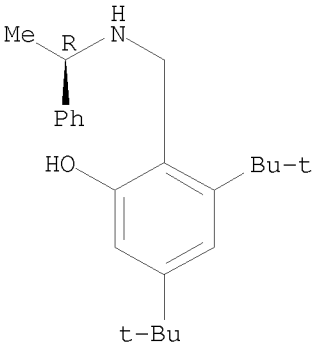


RN 639069-49-1 CAPLUS
CN Phenol, 2-[(decylamino)methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)

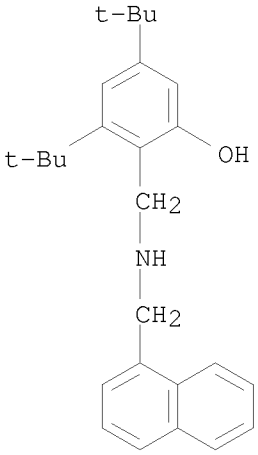


RN 639069-58-2 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[(1R)-1-phenylethyl]amino]methyl]- (CA INDEX NAME)

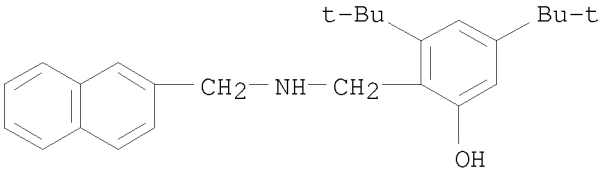
Absolute stereochemistry.



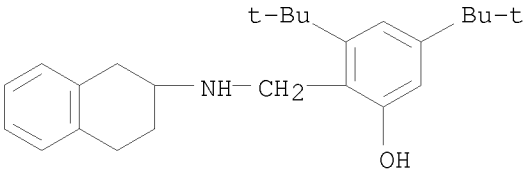
RN 639069-59-3 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(1-naphthalenylmethyl)amino]methyl]-
(CA INDEX NAME)



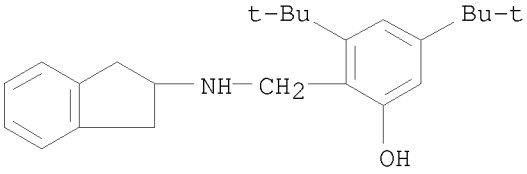
RN 639069-60-6 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(2-naphthalenylmethyl)amino]methyl]-
(CA INDEX NAME)



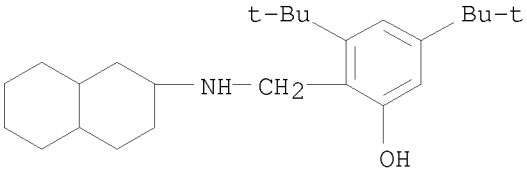
RN 639069-62-8 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(1,2,3,4-tetrahydro-2-
naphthalenyl)amino]methyl]- (CA INDEX NAME)



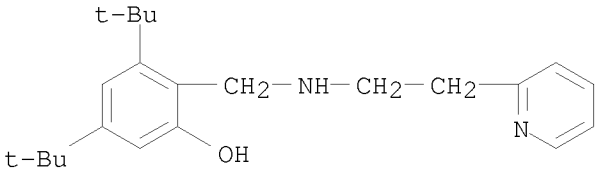
RN 639069-64-0 CAPLUS
CN Phenol, 2-[[(2,3-dihydro-1H-inden-2-yl)amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



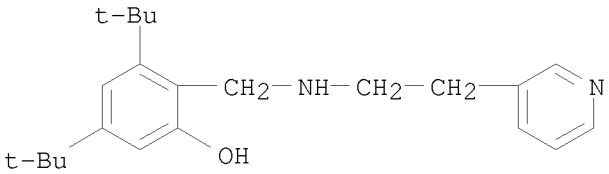
RN 639069-73-1 CAPLUS
CN Phenol, 2-[[(decahydro-2-naphthalenyl)amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



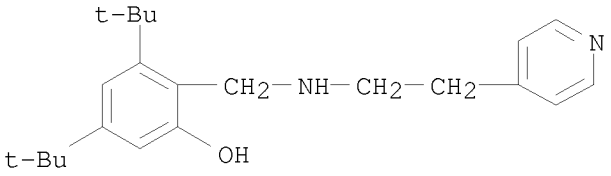
RN 639069-76-4 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[2-(2-pyridinyl)ethyl]amino]methyl]- (CA INDEX NAME)



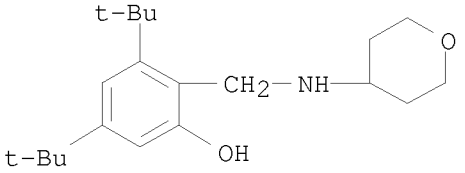
RN 639069-77-5 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[2-(3-pyridinyl)ethyl]amino]methyl]- (CA INDEX NAME)



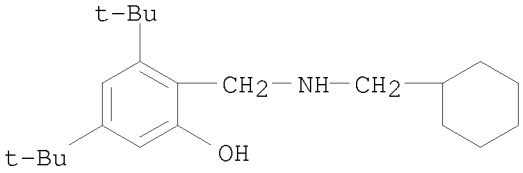
RN 639069-78-6 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[2-(4-pyridinyl)ethyl]amino]methyl]- (CA INDEX NAME)



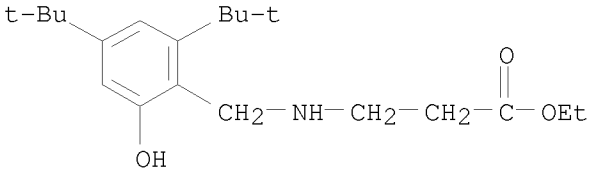
RN 639069-79-7 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(tetrahydro-2H-pyran-4-yl)amino]methyl]- (CA INDEX NAME)



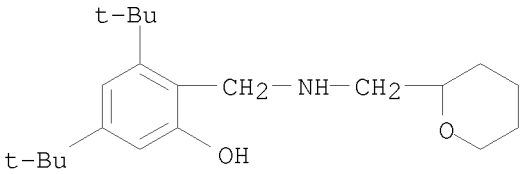
RN 639069-80-0 CAPLUS
CN Phenol, 2-[[(cyclohexylmethyl)amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



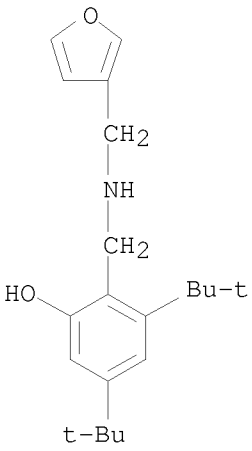
RN 639069-83-3 CAPLUS
CN β-Alanine, N-[[2,4-bis(1,1-dimethylethyl)-6-hydroxyphenyl]methyl]-, ethyl ester (CA INDEX NAME)



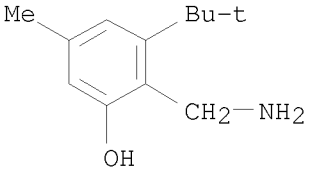
RN 639069-88-8 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[(tetrahydro-2H-pyran-2-yl)methyl]amino]methyl]- (CA INDEX NAME)



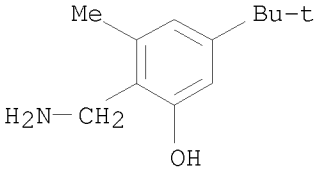
RN 639069-90-2 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(3-furanylmethyl)amino]methyl]- (CA INDEX NAME)



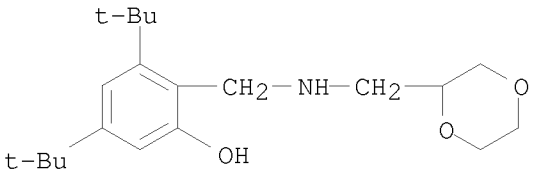
RN 639069-92-4 CAPLUS
CN Phenol, 2-(aminomethyl)-3-(1,1-dimethylethyl)-5-methyl- (CA INDEX NAME)



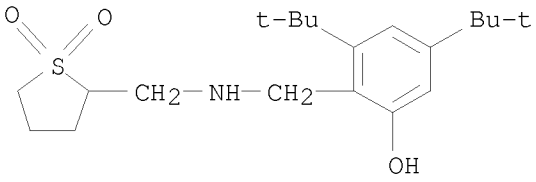
RN 639070-01-2 CAPLUS
CN Phenol, 2-(aminomethyl)-5-(1,1-dimethylethyl)-3-methyl- (CA INDEX NAME)



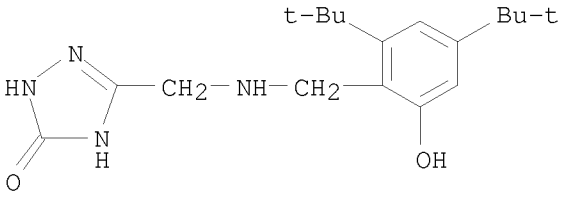
RN 639070-04-5 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(1,4-dioxan-2-ylmethyl)amino]methyl]- (CA INDEX NAME)



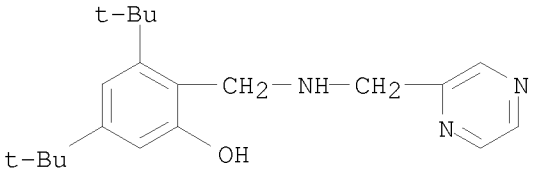
RN 639070-05-6 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[(tetrahydro-1,1-dioxido-2-thienyl)methyl]amino]methyl]- (CA INDEX NAME)



RN 639070-06-7 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[[[[2,4-bis(1,1-dimethylethyl)-6-hydroxyphenyl]methyl]amino]methyl]-1,2-dihydro- (CA INDEX NAME)

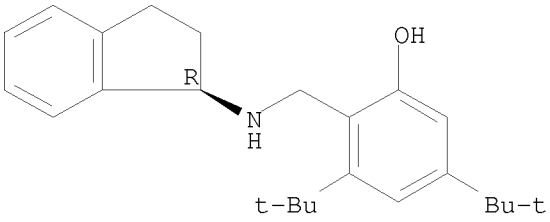


RN 639070-08-9 CAPLUS
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[(2-pyrazinylmethyl)amino]methyl]- (CA INDEX NAME)



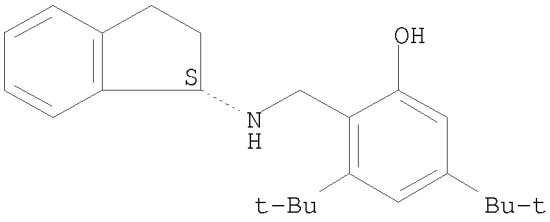
RN 639070-64-7 CAPLUS
CN Phenol, 2-[[[(1R)-2,3-dihydro-1H-inden-1-yl]amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 639070-65-8 CAPLUS
CN Phenol, 2-[[[(1S)-2,3-dihydro-1H-inden-1-yl]amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)

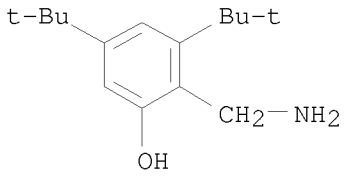
Absolute stereochemistry.



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

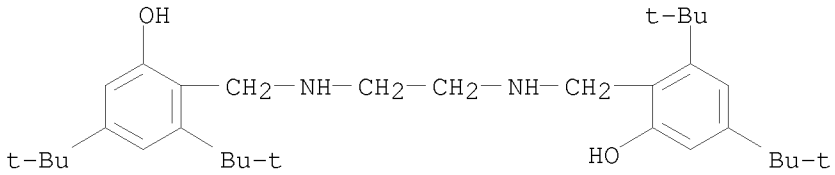
L4 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:857716 CAPLUS
DN 138:197738
TI A structurally characterized monomeric Mn(IV) complex in a discrete N2O4 coordination environment
AU Rajendiran, T. M.; Kampf, Jeff W.; Pecoraro, Vincent L.
CS Department of Chemistry, The University of Michigan, Ann Arbor, MI, 48109-1055, USA
SO Inorganica Chimica Acta (2002), 339, 497-502
CODEN: ICHAA3; ISSN: 0020-1693
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 138:197738
AB From the reaction of Mn(III)(OAc)3 with (3,5-di-tert-butyl-2-hydroxyphenylmethyliminomethyl)3,5-di-tert-butyl-phenol (H2dbpip) in MeCN, dark brown crystals of compound Bis[(3,5-di-tert-butyl-2-hydroxyphenylmethyliminomethyl)3,5-di-tert-butylphenolato]manganese (IV), Mn(IV)(dbpip)2 (1) were obtained upon slow evaporation of the solvent. The structural assignments of 1, that were made in part by elemental anal. and magnetic susceptibility, were confirmed by single crystal x-ray diffraction studies which revealed that compound 1 crystallizes in the monoclinic, space group C2/c with a cell dimensions a = 49.746(8), b = 12.682(2), c 19.497(3) Å,α 90, β 94.240(3), γ 90°. Cyclic voltammetry reveals a quasi reversible redox wave corresponding to the Mn(III)/Mn(IV) couple. The EPR spectrum at 4 K consists of strong and weak signals near g = 2 and 4, resp. A comparison of the EPR spectrum to there obtained for other Mn(IV)N2O4 complexes reveals that 1 is a rare example of an axial Mn(IV) species with

D«hν.
IT 84210-35-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of hydroxyphenylmethyliminomethylphenol)
RN 84210-35-5 CAPLUS
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)

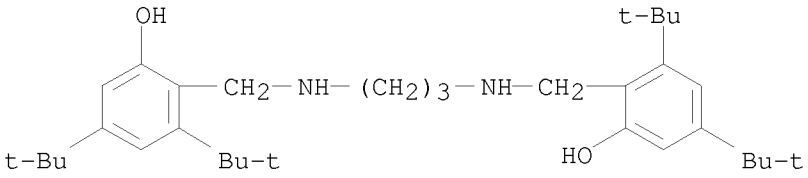


RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2001:615153 CAPLUS
DN 136:5753
TI Single-step synthesis of salans and substituted salans by Mannich condensation
AU Tshuva, E. Y.; Gendeziuk, N.; Kol, M.
CS Raymond and Beverly Sackler Faculty of Exact Sciences, School of Chemistry, Tel Aviv University, Tel Aviv-Jaffa, 69978, Israel
SO Tetrahedron Letters (2001), 42(36), 6405-6407
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 136:5753
AB A convenient route for the synthesis of a variety of salan-type compds. is introduced. The synthesis is based on a single-step Mannich condensation between readily available starting materials: primary or secondary amines, formaldehyde and substituted phenols. This methodol. is suitable for the preparation of chiral salans as well, which may find applications in asym. catalysis.
IT 375793-66-1P 375793-68-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of salans by Mannich condensation)
RN 375793-66-1 CAPLUS
CN Phenol, 2,2'-[1,2-ethanediylbis(iminomethylene)]bis-3,5-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



RN 375793-68-3 CAPLUS
CN Phenol, 2,2'-[1,3-propanediylbis(iminomethylene)]bis[3,5-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

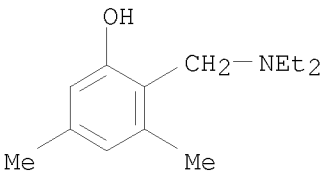


RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

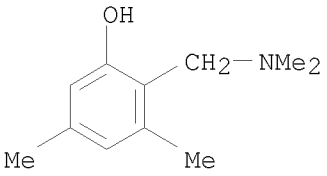
L4 ANSWER 6 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1994:508209 CAPLUS
DN 121:108209
OREF 121:19519a,19522a
TI Preparation of o-(aminoalkyl)phenols
IN Ezaki, Yoichiro
PA Arakawa Chem Ind, Japan
SO Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05331114	A	19931214	JP 1992-164390	19920529
			JP 1992-164390	19920529

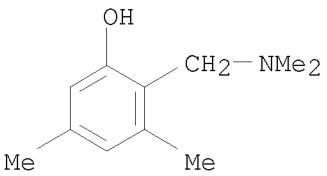
OS CASREACT 121:108209
AB The title compds. are prepared by reaction of phenols having ≥1 unsubstituted o-position, aldehydes or ketones, and secondary amines followed by removing impurities from the reaction mixts. by treatment with alkali metal and/or alkaline earth metal hydroxides. A mixture of aqueous Me2NH, 3,5-dimethylphenol, and aqueous HCHO was kept at 25-35° for 4 h, mixed with toluene, and the organic layer was treated with aqueous NaOH to give 86% 2-(N,N-dimethylaminomethyl)-3,5-dimethylphenol.
IT 38942-39-1P, 2-(N,N-Diethylaminomethyl)-3,5-dimethylphenol
63487-28-5P, 2-(N,N-Dimethylaminomethyl)-3,5-dimethylphenol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from phenol and purification of)
RN 38942-39-1 CAPLUS
CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



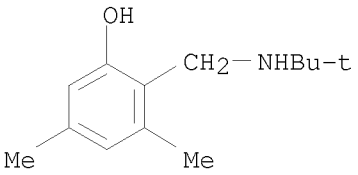
RN 63487-28-5 CAPLUS
CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 7 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1991:562575 CAPLUS
DN 115:162575
OREF 115:27783a,27786a
TI Influence of structure and other characteristics of substitute fuel components in petrol on engine efficiency and pollution
AU Stournas, S.; Lois, E.; Polyssis, P.; Serdari, A.; Swithenbank, J.; Priestman, G. H.; Papachristos, M.
CS Fuels Lubr. Lab., Natl. Tech. Univ., Athens, 106 82, Greece
SO Comm. Eur. Communities, [Rep.] EUR (1991), EUR 13157, 157pp.
CODEN: CECED9; ISSN: 0303-755X
DT Report
LA English
AB Terpenic derivs., a new class of compds., Mannich base phenols, and tertiary polyamines (>60 compds.) were evaluated for their antiknock properties for 4 model gasolines. The effects of these additives on NOx, CO, and HCHO emissions from a test engine were also determined
IT 63487-28-5 136029-09-9
RL: USES (Uses)
(gasoline antiknock additive, mol. structure effect and air pollution in relation to)
RN 63487-28-5 CAPLUS
CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



RN 136029-09-9 CAPLUS
CN Phenol, 2-[[(1,1-dimethylethyl)amino]methyl]-3,5-dimethyl- (CA INDEX NAME)

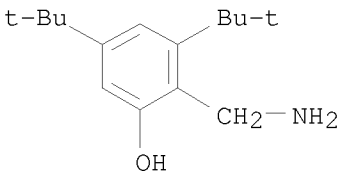


L4 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1988:140707 CAPLUS

DN 108:140707
OREF 108:22935a,22938a
TI Triboelectrifying material for charging electrostatographic toner
IN Fukumoto, Hiroshi; Tanaka, Katsuhiko; Kawagishi, Yoji
PA Canon K. K., Japan; Orient Chemical Industries, Ltd.
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 61160763	A	19860721	JP 1985-819	19850109
JP 06046314	B	19940615		
			JP 1985-819	19850109

AB The triboelectrifying material has on its surface a metal-salicylamine or alkylsalicylamine complex. The complex may be coated on carrier particles, on a developing sleeve, or on a developing doctor blade. An Fe powder may be coated with Co-salicylamine complex to give the title material. The material shows improved durability in providing images with constant d.
IT 84210-35-5D, complexes with transition metals
RL: USES (Uses)
(triboelectrifying agents, for electrostatog. toners, with improved durability)
RN 84210-35-5 CAPLUS
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



L4 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1985:487767 CAPLUS
DN 103:87767
OREF 103:14097a,14100a
TI Cyclohexane-1,3-dione derivatives and their herbicidal compositions and methods
IN Serban, Alexander; Watson, Keith G.; Bird, Graham J.; Farquharson, Graeme J.
PA ICI Australia Ltd. , Australia
SO U.S., 21 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4511391	A	19850416	US 1983-497683	19830524
			AU 1983-4118 A	19830524

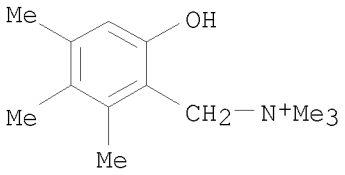
OS MARPAT 103:87767
AB Benzofuranylcyclohexenones and related compds. I [R = halo, NO2, cyano,

OH, (un)substituted alkyl, alkoxy, HO3SNH, etc.; R1 = (un)substituted alkyl, alkenyl, alkynyl; R2 = Ph, alkyl, furoalkyl, alkenyl, alkynyl; R3 = H, halo, cyano, alkyl, alkoxycarbonyl; R4 = H, (un)substituted alkyl, alkenyl, alkynyl, alkylsulfonyl, PhSO2, Bz, inorg. or organic cation; X, X1 = O, S, CH2; at least one of X and X1 is O or S; n = 1-3; n1 = 0-3] were prepared Thus, phenol II (R5 = H) was treated with CH2O and HNMe2 to give II (R5 = CH2NMe2), which was quaternized with MeI and treated with Me2S(O):CH2 to give benzofuran III (R6 = H). III (R6 = H) was carboxylated and condensed with acetone to give III (R6 = CH:CH2COMe), which underwent cyclocondensation with (EtO2C)2CH2 to form cyclohexenoylbenzofuran IV (R7 = H). IV (R7 = H) was acylated with (PrCO)2O to give IV (R7 = COPr), which condensed with EtONH2 to give IV (R7 = CPr:NOEt) (V). At 0.02 kg/ha postemergence, V inflicted 81-99% damage on Echinochola crus-galli, whereas winter wheat and rice were undamaged.

IT 89240-11-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, benzofuran by)

RN 89240-11-9 CAPLUS

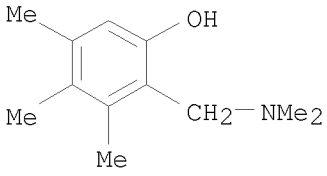
CN Benzenemethanaminium, 6-hydroxy-N,N,N,2,3,4-hexamethyl-, iodide (9CI) (CA INDEX NAME)



IT 89240-10-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and quaternization of)

RN 89240-10-8 CAPLUS

CN Phenol, 2-[(dimethylamino)methyl]-3,4,5-trimethyl- (CA INDEX NAME)



L4 ANSWER 10 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

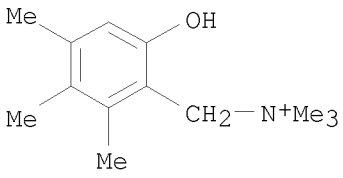
AN 1985:37229 CAPLUS

DN 102:37229

OREF 102:5799a,5802a

TI The crystal structures of 4,4'-bipyridinium μ-(4,4'-

bipyridine)bis[diaquatetranitratoneodymate(III)]-tris(4,4'-bipyridine) and a second monoclinic form of triaquatrinitratoholmium(III)-bis(4,4'-bipyridine)
AU Weakley, Timothy J. R.
CS Dep. Chem., Dundee Univ., Dundee, DD1 4HN, UK
SO Inorganica Chimica Acta (1984), 95(6), 317-22
CODEN: ICHAA3; ISSN: 0020-1693
DT Journal
LA English
AB The 1st title compound is monoclinic, space group P21/c, with a 18.723(10), b 10.720(6), c 18.027(10) Å, and β 94.43(5)°; Z = 2; R = 0.066 for 4931 data. The 2nd title monoclinic form has space group P21/c, with a 15.830(10), b 21.44(3), c 15.70(3) Å, and β 100.4(2)°, Z = 8; R = 0.091 for 2335 film data. In the 1st compound pairs of Nd atoms are bridged across a crystal inversion center by a 4-bipy ligand, and 10-coordination is completed by 4 monodentate NO3, 3 bidentate NO3, and 2 H2O ligands, with bond lengths Nd-N 2.70, Nd-OH2(average) 2.44, and Nd-O(NO3, average) 2.56 Å. The 2nd compound has a variant of the previously-reported monoclinic [Y(NO3)3(H2O)3].2(4-bipy) structure, with doubling of the unit cell on a but with essentially no change in the geometry and orientation of the 9-coordinate complex. In both compds. the noncoordinated, nonprotonated 4-bipy N atoms form H bonds with ligand H2O.
IT 89240-11-9
RL: PRP (Properties)
(structure of)
RN 89240-11-9 CAPLUS
CN Benzenemethanaminium, 6-hydroxy-N,N,N,2,3,4-hexamethyl-, iodide (9CI) (CA INDEX NAME)



● I⁻

L4 ANSWER 11 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1984:121043 CAPLUS
DN 100:121043
OREF 100:18425a,18428a
TI Herbicidal cyclohexane-1,3-dione derivatives
IN Serban, Alexander; Watson, Keith Geoffrey; Bird, Graham John; Farquharson, Graeme John
PA ICI Australia Ltd. , Australia
SO Eur. Pat. Appl., 86 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI EP 95330 A1 19831130 EP 1983-302861 19830519
EP 95330 B1 19871119
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE
AU 1982-4118 A 19820524
AU 8314477 A 19831201 AU 1983-14477 19830511
AU 560842 B2 19870416
AU 1982-4118 A 19820524
ZA 8303398 A 19840229 ZA 1983-3398 19830511
AU 1982-4118 A 19820524
AT 30913 T 19871215 AT 1983-302861 19830519
AU 1982-4118 A 19820524
EP 1983-302861 A 19830519
HU 31922 A2 19840628 HU 1983-1783 19830520
HU 189285 B 19860630
AU 1982-4118 A 19820524
JP 58213769 A 19831212 JP 1983-89300 19830523
JP 05026788 B 19930419
AU 1982-4118 A 19820524
CA 1202634 A1 19860401 CA 1983-428746 19830524
AU 1982-4118 A 19820524

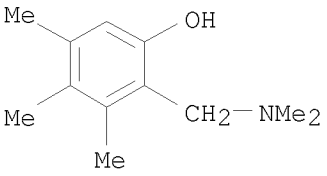
OS MARPAT 100:121043

AB Cyclohexanediones I [R = H, (un)substituted alkyl, Ph, SO3H, SO2Ph; R1 = alkyl, fluoroalkyl, alkenyl, alkynyl, Ph; R2 = (un)substituted alkyl, Ph; R3 = H, halogen, cyano, alkyl, alkoxycarbonyl; R4 = substituted Ph] were prepared Thus, piperonal was treated with Me2CO and CH2(CO2Et)2 to give II (R5 = H) which was acylated with (EtCO)2O and treated with EtONH2.HCl to give II (R5 = CEt:NOEt)(III). At 0.2 kg/ha pre-emergence III gave 100% kill of Echinochloa crus-galli.

IT 89240-10-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and quaternization of)

RN 89240-10-8 CAPLUS

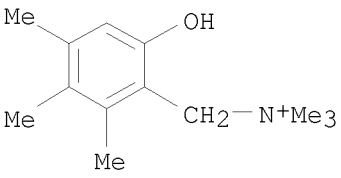
CN Phenol, 2-[(dimethylamino)methyl]-3,4,5-trimethyl- (CA INDEX NAME)



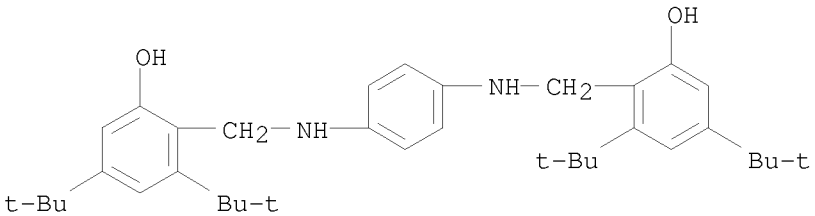
IT 89240-11-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with dimethylsulfoxium methylide)

RN 89240-11-9 CAPLUS

CN Benzenemethanaminium, 6-hydroxy-N,N,N,2,3,4-hexamethyl-, iodide (9CI) (CA INDEX NAME)

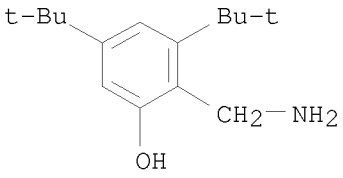


L4 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1983:163553 CAPLUS
DN 98:163553
OREF 98:24795a,24798a
TI Study of the effectiveness of inhibitors in oxidation of jet fuel in a closed volume
AU Kovalev, G. I.; Denisov, E. T.; Nikonova, A. G.; Gerasimova, A. V.; Burachevskaya, I. I.
CS Otd. Inst. Khim. Fiz., Chernogolovka, USSR
SO Deposited Doc. (1981), VINITI 443-82, 23 pp. Avail.: VINITI
DT Report
LA Russian
AB Extensive tests were conducted to study the antioxidative and heat stabilizing activity of amines, alkylphenols, aminophenols, and organophosphorus and organosulfur compds. in T6 jet aircraft fuel. The most effective were aminophenols. At 0.003 weight% concentration their ability to suppress the autoxidn. of T 6 at 170° exceeded the ability of Ionol [128-37-0]. The best antioxidant in this series was 4-phenylaminophenol [122-37-2].
IT 85404-01-9
RL: USES (Uses)
(antioxidants-heat stabilizers, for jet aircraft fuels)
RN 85404-01-9 CAPLUS
CN Phenol, 2,2'-[1,4-phenylenebis(iminomethylene)]bis[3,5-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 13 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1983:53306 CAPLUS
DN 98:53306
OREF 98:8181a,8184a
TI The use of sterically hindered benzylamines in the Sommelet reaction
AU Stokker, G. E.; Schultz, E. M.

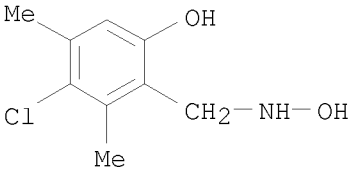
CS Merck Sharp Dohme Res. Lab., West Point, PA, 19486, USA
SO Synthetic Communications (1982), 12(11), 847-53
CODEN: SYNCAV; ISSN: 0039-7911
DT Journal
LA English
OS CASREACT 98:53306
AB Amines I (R = H, Me; R1 = H, halo, Me; R2 = H, alkyl, OMe; R3 = alkyl, H, Cl; R4 = H, alkyl, Cl, OMe) were converted to the resp. aldehydes II. Thus, I (R = R2 = R4 = H, R1 = iodo, R3 = CMe3) hydrochloride was heated with hexamethylenetetramine in aqueous HOAc to give II.
IT 84210-35-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(Sommelet reaction of)
RN 84210-35-5 CAPLUS
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



L4 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1982:142446 CAPLUS
DN 96:142446
OREF 96:23413a,23416a
TI 2-Hydroxylaminomethyl phenols
IN Haviv, Fortuna
PA Abbott Laboratories, USA
SO U.S., 5 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

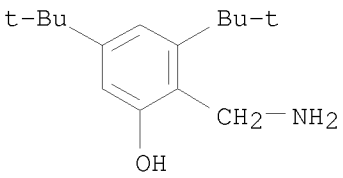
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4312887	A	19820126	US 1978-954699	19781025
			US 1978-954699 A	19781025

OS CASREACT 96:142446; MARPAT 96:142446
AB Salicylaldehydes were converted to phenols I (R and R2 are H, alkyl, alkoxy, Cl; R1 = Cl, alkyl, alkoxy; R3 = H, halo, alkyl, alkoxy, alkylthio, CF3), which exhibited diuretic and antiinflammatory activity. Thus, 3,5-Cl(Me3C)C6H3CHO was oximated and the oxime product was reduced by NaB(CN)H3 to give I (R1 = CMe3, R3 = Cl, R = R2 = H).
IT 81322-69-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and diuretic activity of)
RN 81322-69-2 CAPLUS
CN Phenol, 4-chloro-2-[(hydroxyamino)methyl]-3,5-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



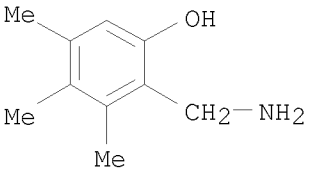
● HCl

L4 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1980:620454 CAPLUS
DN 93:220454
OREF 93:35187a,35190a
TI 2-(Aminomethyl)phenols, a new class of saluretic agents. 1. Effects of nuclear substitution
AU Stokker, G. E.; Deana, A. A.; DeSolms, S. J.; Schultz, E. M.; Smith, R. L.; Cragoe, E. J., Jr.; Baer, J. E.; Ludden, C. T.; Russo, H. F.; et al.
CS Merck Inst. Ther. Res., West Point, PA, 19486, USA
SO Journal of Medicinal Chemistry (1980), 23(12), 1414-27
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 93:220454
AB A series of .apprx.100 2-(aminomethyl)phenols was synthesized and tested in rats and dogs for saluretic and diuretic activity; several were highly active on i.v. or oral administration. The most active were 4-alkyl-6-halo derivs., especially 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenol (I). I also had significant antihypertensive, topical saluretic, and antiinflammatory activity.
IT 51571-04-1P 51571-09-6P 75551-86-9P
75552-02-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as potential diuretic or saluretic agent)
RN 51571-04-1 CAPLUS
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)-, hydrochloride (9CI) (CA INDEX NAME)



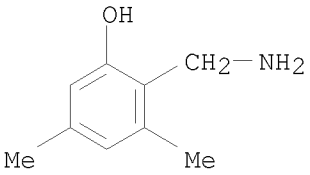
● HCl

RN 51571-09-6 CAPLUS
CN Phenol, 2-(aminomethyl)-3,4,5-trimethyl-, hydrochloride (9CI) (CA INDEX NAME)



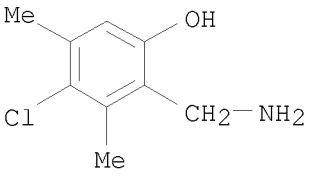
● HCl

RN 75551-86-9 CAPLUS
CN Phenol, 2-(aminomethyl)-3,5-dimethyl-, hydrochloride (6CI, 9CI) (CA INDEX NAME)



● HCl

RN 75552-02-2 CAPLUS
CN Phenol, 2-(aminomethyl)-4-chloro-3,5-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 16 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1980:76524 CAPLUS
DN 92:76524
OREF 92:12611a,12614a
TI 3,4-Dihydro-2H-1,3-benzoxazin-2-one derivatives
IN Arct, Jacek; Jakubska, Elzbieta; Olszewska, Grazyna
PA Politechnika Warszawska, Pol.
SO Pol., 3 pp.
CODEN: POXXA7
DT Patent

LA Polish
FAN.CNT 1

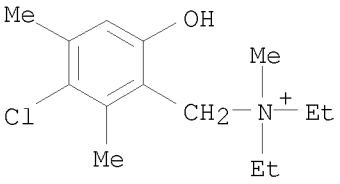
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	PL 100342	B1	19780930	PL 1975-185918	19751223
				PL 1975-185918 A	19751223

AB I [R, R1, R2 (same or different) = H, Cl, C1-5 alkyl, aryl, alkoxy, NO2, cyano, sulfonamido] were prepared by heating II [R3-5 (same or different) = C1-4 alkyl, X = Cl, alkyl or aryl sulfate, or 2-sulfonate] with an alkali cyanide at 70-140° 15-60 h in a polar solvent (MeNO2, MeCN, MeCOEt, DMF). Thus, 0.1 Mol KCN was added to 0.1 Mol III in 300 cc MeNO2, and the mixture refluxed 35 h to give 63% IV.

IT 72724-29-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring closure of, with sodium cyanide)

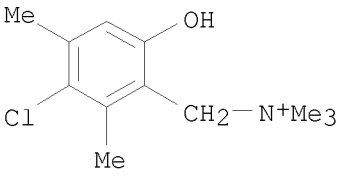
RN 72724-29-9 CAPLUS

CN Benzenemethanaminium, 3-chloro-N,N-diethyl-6-hydroxy-N,2,4-trimethyl-, chloride (9CI) (CA INDEX NAME)

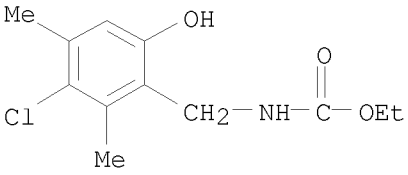


● Cl^-

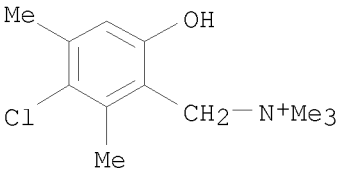
L4 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:509299 CAPLUS
DN 89:109299
OREF 89:16837a,16840a
TI Conversion of Mannich phenol bases; III. Synthesis and transformations of 3,4-dihydro-2H-1,3-benzoxazin-2-one derivatives
AU Arct, J.; Jakubska, E.; Olszewska, G.
CS Inst. Org. Chem. Technol., Warsaw Tech. Univ., Warsaw, Pol.
SO Synthetic Communications (1978), 8(3), 143-9
CODEN: SYNCAV; ISSN: 0039-7911
DT Journal
LA English
OS CASREACT 89:109299
AB Phenols I (R1, R2 = H, Me, Cl) cyclized with KOCN to give 38-78% II, alcoholysis of which gave 86-99% III.
IT 63616-12-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with cyanate, dihydrobenzoxazinone derivative from)
RN 63616-12-6 CAPLUS
CN Benzenemethanaminium, 3-chloro-6-hydroxy-N,N,N,2,4-pentamethyl- (CA INDEX NAME)



IT 67275-17-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 67275-17-6 CAPLUS
CN Carbamic acid, [(3-chloro-6-hydroxy-2,4-dimethylphenyl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)

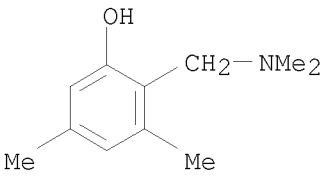


L4 ANSWER 18 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1977:484914 CAPLUS
DN 87:84914
OREF 87:13507a,13510a
TI Conversions of Mannich phenol bases; II. Synthesis of 2-thioxo-2H-3,4-dihydro-1,3-benzoxazine derivatives
AU Arct, Jacek; Jakubska, Elzbieta; Olszewska, Grazyna
CS Inst. Org. Chem. Technol., Warsaw Tech. Univ., Warsaw, Pol.
SO Synthesis (1977), (5), 314-15
CODEN: SYNTBF; ISSN: 0039-7881
DT Journal
LA English
AB Benzoxazines I (R = 6-Me, 6-Cl, 6-Cl-7-Me, 5,7-Me2-6-Cl, 6,7-Cl2) were prepared in 49-74% yield by reaction of the corresponding o-hydroxybenzyltrimethylammonium salt with KSCN.
IT 63616-12-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with potassium thiocyanate)
RN 63616-12-6 CAPLUS
CN Benzenemethanaminium, 3-chloro-6-hydroxy-N,N,N,2,4-pentamethyl- (CA INDEX NAME)



L4 ANSWER 19 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1977:468113 CAPLUS
DN 87:68113
OREF 87:10837a,10840a
TI Sulfones as chemical carriers of substances with germicidal activity. VIII: Sulfonyl derivatives of the Mannich bases of quinaldine, pyrrole and phenol
AU Messinger, Paul; Gompertz, Judith
CS Inst. Pharm. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.
SO Archiv der Pharmazie (Weinheim, Germany) (1977), 310(3), 249-55
CODEN: ARPMAS; ISSN: 0365-6233
DT Journal
LA German
OS CASREACT 87:68113
AB 4-MeC6H4SO2CH2CHRCH2NMe2.HCl (R = 2-quinolyl) was prepared by treating RCH2CH2NMe2 with 4-MeC6H4SO2H and aminomethylating RCH2CH2SO2C6H4Me-4. I (NR1R2 = NMe2, piperidino) were obtained by treating 2-dimethylaminomethyl-1-methylpyrrole methiodide with NaSO2Ph and aminomethylating 1-methyl-2-phenylsulfonylmethylpyrrole. II (NR1R2 = NMe2, piperidino, morpholino) were similarly obtained from 2,4,6-HO(Me)2C6H2CH2NMe2.MeI. 4-MeC6H4SO2CH(CH2Bz)C6H3(OH)CH2NEt2.HCl-4,3 was prepared by aminomethylating BzCH:CHC6H4OH-4 and treating 2,4-HO(BzCH:CH)C6H3CH2NEt2.HCl with 4-MeC6H4SO2H. 4-MeC6H4SO2CHPhCH2COC6H3(OH)CH2NEt2.HCl-4,3 was similarly obtained from PhCH:CHCOC6H4OH-4.
IT 63487-28-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with toluenesulfinate)
RN 63487-28-5 CAPLUS
CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1974:120533 CAPLUS
DN 80:120533
OREF 80:19395a,19398a
TI Treating edema and hypertension using certain 2-aminoethylphenols
IN Cragoe, Edward J., Jr.; Schultz, Everett M.
PA Merck and Co., Inc.
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3794734	A	19740226	US 1971-120730	19710303
			A	
US 3979361	A	19760907	US 1975-600990	19750801
			US 1971-120730 A2	19710303
			US 1974-444200 A2	19740220

	US 4044153	A	19770823	US 1976-684138		19760507
				US 1971-120730	A2	19710303
				US 1974-444200	A2	19740220
				US 1975-600990	A1	19750801

PATENT FAMILY INFORMATION:

FAN 1977:29478

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	US 3979361	A	19760907	US 1975-600990		19750801
				US 1971-120730	A2	19710303
				US 1974-444200	A2	19740220
	US 3794734	A	19740226	US 1971-120730		19710303
					A	
	US 4044153	A	19770823	US 1976-684138		19760507
				US 1971-120730	A2	19710303
				US 1974-444200	A2	19740220
				US 1975-600990	A1	19750801

FAN 1977:551847

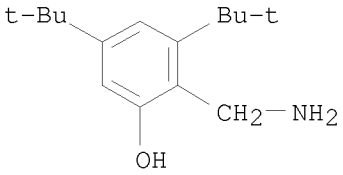
	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	US 4044153	A	19770823	US 1976-684138		19760507
				US 1971-120730	A2	19710303
				US 1974-444200	A2	19740220
				US 1975-600990	A1	19750801
	US 3794734	A	19740226	US 1971-120730		19710303
					A	
	US 3979361	A	19760907	US 1975-600990		19750801
				US 1971-120730	A2	19710303
				US 1974-444200	A2	19740220

AB 2-(Aminomethyl)phenols (I; e.g., R = R2 = R3 = Cl, R1 = H; R = Me, R1 = R3 = H, R2 = Me3C; R = H, R1 = R3 = MeO, R2 = Cl), useful in the treatment of adema and hypertension, were prepared Thus, treatment of 2,4,5-Cl3C6H2OH and ClCH2-CONHCH2OH with H2SO4 gave the amide (II) which, when treated with ethanolic HCl, gave I (R = R2 = R3 = Cl, R1 = H). About 24 I were prepared similarly.

IT 51571-04-1P 51571-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51571-04-1 CAPLUS

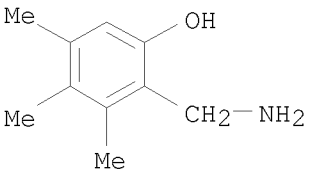
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 51571-09-6 CAPLUS

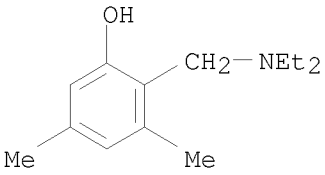
CN Phenol, 2-(aminomethyl)-3,4,5-trimethyl-, hydrochloride (9CI) (CA INDEX NAME)



L4 ANSWER 21 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1972:514037 CAPLUS
DN 77:114037
OREF 77:18785a,18788a
TI Aminomethyl substituted phenol esters
IN Gablech, Miloslav; Major, Milan
SO Czech., 2 pp.
CODEN: CZXXA9
DT Patent
LA Czech
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 142844		19710915	CS 1968-8500	19681213

AB The title esters are prepared by esterification of phenols with acid anhydrides under conditions which prevent decomposition of the resulting Mannich bases. Thus, 2-[(diethylamino)methyl]-3,5-dimethylphenol, obtained by aminomethylation of m-xylenol, was heated (1 mole) with 1.2 moles Ac2O 30 min at 50° with simultaneous in vacuo distillation of AcOH formed and excess Ac2O separated in vacuo to give 90% 2-[(diethylamino)methyl]-3,5-dimethylacetoxybenzene.
IT 38942-39-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(acetylation of, with acetic anhydride)
RN 38942-39-1 CAPLUS
CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)

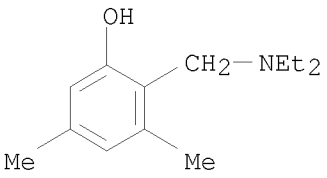


L4 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1961:135955 CAPLUS
DN 55:135955
OREF 55:25561g-h
TI Diazo materials for prints
IN Slimowicz, Chester Edward

PA General Aniline & Film Corp.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 867432		19610510	GB 1959-25553	19590724
	DE 1160732			DE	

AB A 2-component system of a light-sensitive diazo compound containing a Ph group substituted by a heterocyclic nitrogenous ring containing a hetero-O and a coupler compound, which is a derivative of a PhOH or resorcinol, produces prints with little background discoloration. The usual S stabilizers are eliminated and storage with Ag van dyke prints is thus made practical. Cf. CA 37, 13425; 55, 2324d.
IT 38942-39-1
    (Derived from data in the 6th Collective Formula Index (1957-1961))
RN 38942-39-1 CAPLUS
CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 23 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1961:135954 CAPLUS
DN 55:135954
OREF 55:25560a-i,25561a-g
TI Methine dyes
IN Ficken, Geoffrey Ernest; Kendall, John D.
PA Ilford Ltd.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 870753		19610621	GB 1957-21185	19570704

AB Cyanine dyes containing the 3,4-diazaindene ring system are useful as optical sensitizers in photographic Ag halide emulsions. Dyes were produced with the general formula A and B, where Z' is Q.N(R'''').(CH:Z)n.C:CH(CH:CH)m or 4-AN(A')C6H4CH:CH, A, A', R, R' are lower alkyl groups, R'''' is a lower alkyl, hydroxyalkyl or aralkyl group, R''' is a lower alkyl or aralkyl group, n and m are 0 or 1, X' is Q'.C(:O).C:CHCH:, Z is CH or N, Q is the residue of a 5- or 6-membered heterocyclic ring, Q' is the residue of a keto-methylene nucleus, X is an acid radical, and Y is H or a lower alkyl. 2-Hydrazinopyridine (115 g.), 125 ml. iso-PrCOMe and 300 ml. dry benzene were refluxed, the H2O formed removed by azeotropic distillation, the benzene distilled, and the residual oil heated with 1 g. ZnCl2 at 250° until NH3 evolution ceased, gave a product, b6 115°, which was redistd. The fraction b6 109-32° was extracted with ligroine (b. 60-80°) to give 1,1,2-trimethyl-3,4-diazaindene (I), m.p. 77-8° (cyclohexane). I (2.0 g.), 2.0 ml. MeI, and 10 ml. acetone

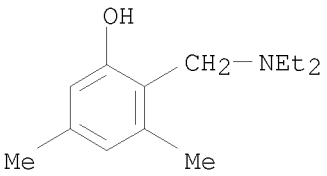
were refluxed for 0.5 hr. to give 1,1,2-trimethyl-3,4-diazaindene-4-MeI (II), m.p. 218-19° (decompose) (EtOH). 2-Methylthiobenzothiazole-MeI (III) (1.62 g.) and 1.52 g. II were refluxed in 30 ml. EtOH containing 1.0 ml. Et3N for 3 hrs. to give (1,1,4-trimethyl-3,4-diaza-2-indene)(3-methyl-2-benzothiazole)methinecyanine iodide, m. 313-14° (decompose) (MeOH) which extended the sensitivity of AgCI emulsions to 4950 A., maximum 4700 A. Similarly prepared were (4-ethyl-1,1-dimethyl-3,4-diaza-2-indene)(3-ethyl-2-benzothiazole)methinecyanine iodide, m. 318-19° (decomposition) (MeOH), and (1,1,4-trimethyl-3,4-diaza-2-indene)(1-methyl-2-quinoline)methinecyanine perchlorate, m. 250-1° (MeOH-HOCH2CH2OMe), both extending the sensitivity of AgCl from 4350 to 5800 A. with maximum 5300 A. 2-(2-Acetylanilinovinyl)benzoxazole-MeI (IV) (0.84 g.), 0.60 g. II and 5.0 ml. pyridine were refluxed for 0.25 hr. to give (1,1,4 - trimethyl - 3,4- diaza-2 - indene)(3-methyl- 2 - benzoxazole)trimethinecyanine iodide, m. 268-9° (decompose) (MeOH-HOCH2CH2OMe), extending the sensitivity of Ag iodobromide to 6000 A., maximum 5200 and 5600 A. Similarly, (1,1,4-trimethyl-3,4-diaza-2-indene)(1,3,3-trimethyl-2-indolenine)trimethinecyanine perchlorate, m. 271-2° (decompose) (MeOH) was produced, extending the sensitivity of Ag iodobromide to 6250 A., maximum 5900 and 6280 A. HC(OEt)3 (1.6 ml.), 0.76 g. II, and 0.71 g. 3-methyl-1-phenyl-5-pyrazolone in 5 ml. pyridine were refluxed 0.5 hr. to give 4-(2,4-dihydro-1,1,4-trimethyl-3,4-diazainden-2-ylideneethylidene)-3-methyl-1-phenyl-5-pyrazolone, m. 251-2° (EtOH), extending sensitivity of AgCl emulsions from 4600-5550 A., maximum 5350 A. 5-Ethoxymethylene-3-ethyl-2-thio-4-thiazolidinone (V) (0.54 g.) and 0.76 g. II were refluxed in 10 ml. EtOH and 1.0 ml. Et3N for 20 min. to give 5-(2,4-dihydro-1,1,4-trimethyl-3,4-diazainden-2-ylideneethylidene)-3-ethyl-2-thio-4-thiazolidinone, m. 257-9° (MeOH-HOCH2CH2OMe), extending the sensitivity of Ag iodobromide to 6300 A., maximum 6000 A. p-Dimethylaminobenzaldehyde (0.30 g.) and 0.60 g. II were refluxed in 5 ml. pyridine containing 1 drop piperidine for 1.5 hr.to give 1,1-dimethyl-2-(p-dimethylaminostyryl)diazaindene-4-MeI, m. 272-3° (decompose) (MeOH), extending the sensitivity of Ag iodobromide to 6200 A., maximum 5800 A. 4-Methyl-2-methylthiothiazole-MeI and 0.79 g. II-EtI were refluxed in 10 ml. EtOH containing 0.5 ml. Et3N for 1 hr. and added to aqueous NaClO4 to give (4-ethyl-1,1-dimethyl-3,4-diaza-2-indene)(3,4-dimethyl-2-thiazole)methinecyanine perchlorate, m. 203-4° (EtOH), extending the range of AgCl from 4300 to 4750 A., maximum 4600 A. Similarly prepared was (4-ethyl-1,1-dimethyl - 3,4-diaza - 2 -indene)(3-methyl-4-phenyl-2-thiazole)methinecyanine perchlorate, m. 289-90° (decompose) (MeOH), sensitivity of AgCl extended to 4850 A., maximum 4650 A. 2-(2-Ethylthiovinyl)quinoline-MeI (0.71 g.) and 0.60 g. II were refluxed in 10 ml. EtOH containing 0.5 ml. Et3N for 0.5 hr. to give (1,1,4-trimethyl-3,4-diaza-2-indene)(1-methyl-2-quinoline)trimethinecyanine iodide, m. 250-1° (decompose) (EtOH) and extended the sensitivity of Ag iodobromide from 5850 to 6550 A. with maximum 6300 A. Similarly produced were (1,1,4-trimethyl-3,4-diaza-2-indene)(1-methyl-4-quinoline)trimethinecyanine iodide, m. 298° (decompose) (MeOH); and (1,1,4-trimethyl-3,4-diaza-2-indene-(3-methyl-2-benzothiazole)trimethinecyanine iodide, m. 269-70° (MeOH), which extended the sensitivity of Ag iodobromide to 6400 A., maximum 6050 A. 1,1-Diethyl-2-methyl-3,4-diazaindene (VI) (0.66 g.) and 0.80 g. p-MeC6H4SO3Me (VII) were heated at 100° for 20 min., refluxed in 10 ml. pyridine with 1.1 g. IV for 1 hr., and poured into aqueous NaClO4. (1,1-Diethyl-4-methyl-3,4-diaza-2-indene)(3-methyl-2-benzoxazole)trimethinecyanine perchlorate separated, m. 191° (EtOH). Similarly produced was (1,1-diethyl-4-methyl-3,4-diaza-2-indene)(3-methyl-2-benzothiazole)trimethinecyanine perchlorate, m. 203-3.5° (EtOH),

extending Ag iodobromide to 6250 A. with maximum 6000 A. A mixture of 0.70 g. VI, 0.70 g. 2-methylthioquinoline, and 1.6 g. VII was fused at 140° for 1.5 hr. and refluxed for 0.5 hr. with 5 ml. pyridine. Upon addition of aqueous NaClO4, (1,1-diethyl-4-methyl-3,4-diaza-2-indene)(1-methyl-2-quinoline)methinecyanine perchlorate precipitated, m. 207-8° (EtOH). A solution of 1.58 g. 1,1,2,5-tetramethyl-3,4-diazaindene-4-MeI (VIII) and 1.62 g. III in 20 ml. EtOH was refluxed with 1.0 ml. Et3N for 0.5 hr. (1,1,4,5-Tetramethyl-3,4-diaza-2-indene)(3 - methyl - 2 - benzothiazole)methinecyanine iodide separated, m. 347-9° (decompose) (MeOH-HOCH2CH2OMe) and extended the sensitivity of AgCl to 5000 A. with maximum 4700 A. A mixture of 0.63 g. VIII and 0.54 g. IV was refluxed in 15 ml. pyridine for 0.5 hr. to give (1,1,4,5-tetramethyl-3,4 - diaza - 2 - indene)(3 - methyl - 2 - benzoxazole)trimethinecyanine iodide, m. 301-2° (decompose) (HOCH2CH2OMe); Ag iodobromide sensitivity was extended to 5800 A., maximum 5650 A. 1,1,2,7-Tetramethyl-3,4-diazaindene-4-MeI (IX) (0.63 g.) and 0.84 g. IV were refluxed in 5 ml. pyridine to give (1,1,4,7 - tetramethyl-3,4- diaza-2 - indene)(3-methyl-2-benzoxazole)trimethinecyanine iodide, m. 283-4° (MeOH) which extended Ag iodobromide sensitivity to 6050 A., maximum 5600 A. Similarly prepared was (1,1,4,7-tetramethyl-3,4-diaza-2-indene)(3-methyl-2-benzothiazole)trimethinecyanine iodide, m. 271-2° (MeOH) and extending Ag iodobromide sensitivity to 6400 A., maximum 5650 A., and 6000 A. A solution of 0.64 g. IX and 0.44 g. V in 10 ml. EtOH was refluxed with 0.5 ml. Et3N for 0.5 hr. to give 5-(2,4-dihydro-1,1,4,7 - tetramethyl- 3,4 - diazainden - 2 - ylideneethylidene)3-ethyl-2-thio-4-thiazolidinone, m. 297-8° (decompose) (HOCH2CH2OMe), which extended the sensitivity of a Ag iodobromide emulsion to 6350 A. with maximum 5600 and 6000 A.

IT 38942-39-1, Phenol, 2-(diethylaminomethyl)-3,5-dimethyl-
(in diazotype process)

RN 38942-39-1 CAPLUS

CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 24 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1961:93325 CAPLUS

DN 55:93325

OREF 55:17572c-i,17573a-b

TI Structure of synthetic resins. VIII. The preparation of 3,5-disubstituted 2-hydroxybenzaldehydes

AU Zigeuner, G.; Jellinek, K.

CS Univ. Graz, Austria

SO Monatshefte fuer Chemie (1959), 90, 297-305
CODEN: MOCMB7; ISSN: 0026-9247

DT Journal

LA Unavailable

AB cf. CA 54, 8690f. The following (ArCH2)2NH (I) were prepared by heating the corresponding phenol with (CH2)6N4 (II) [Ar, reaction time (hrs.), reaction temperature, g. phenol, g. II, % yield, crystallization solvent, and m.p.

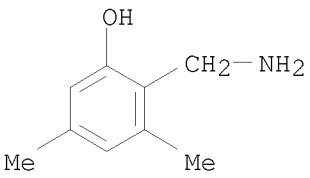
listed]: 5,2,3,6-Cl(OH)(Me2CH)2C6H (III), 2, 130°, 18.4, 15, 87, EtOH, 126°; 5,2,3,6-Br(OH)Me2C6H (IV), 2, 130°, 10, 7, 82, EtOH, 180°; 2,3,6-HO(Me2CH)MeC6H2 (V), 2, 125°, 6.15, 5.13, 68, EtOH, 100°; 2,5-HOMeC6H3 (VI), 3-4, 105°, 20, 2.6, -, xylene, 171°; 2,4,6-HOMe2C6H2 (VII), 3/4, 110°, 3, 1.2, -, EtOH, 181°; 2,3,6-HOMe2C6H2 (VIII), 2, 130°, 5, 11, 90, EtOH, 150°. Treatment of 4 g. 2,4,6-HOMe2C6H2CHO with 2 g. N2H4.H2O in EtOH produced the corresponding aldazine, m. 232° (alc.-H2O), 3 g. of which was reduced with 20 g. Zn powder in 260 mL. boiling EtOH and 30 mL. AcOH to VII. PhOH (10 g.), 4 g. H3BO3, and 5 g. II in 40 mL. (CH2OH)2 boiled 2 h., poured into H2O, the precipitate crystallized several times from dioxane gave a H3BO3 salt, m. 206-10°, saponified with 3 mL. concentrated HCl in 7 mL. EtOH, followed by NaOH, to I (Ar = o-HOC6H4), m. 161°. The following p-MeC6H4NHCH2Ar were prepared by heating the corresponding I 2 h. with p-toluidine (IX) (starting compound, reaction temperature, crystallization solvent, and m.p. listed): III, 120°, -, 110°; IV, 120°, cyclohexane, 137°; V, 160°, ligroine, 106°; VI, 160°, cyclohexane, 106°. A mixture of 4.7 g. 2,3,5-HOMe2C6H2CHO (X) and 6 g. 2,3,5-HOMe2C6H2CH2NH2.HCl, heated 1 h. with 2.5 g. NaHCO3 in 6 mL. EtOH, yielded 2,3,5-HOMe2C6H2CH NCH2C6H2Me2OH-3,5,2 (XI), m. 149° (MeOH); this compound heated 4 h. at 160° with IX formed 2,3,5-HOMe2C6H2CH2NHC6H4Me-p, m. 92°, and 2,3,5-HOMe2C6H2CH:NC6H4Me-p, m. 45° (MeOH); the latter compound was also obtained from IX and X at 180°. A mixture of 78 g. 3,5,4-Me2ClC6H2OH, 45 g. AcNH2, and 22.5 g. paraformaldehyde, saturated with HCl, gave after 3 days 5,2,4,6-Cl(OH)Me2C6HCH2NHAc, m. 175° (EtOH), hydrogenated over Raney Ni to 2,4,6-HOMe2C6H2NHAc, m. 135° (C6H6); saponification of this compound by 8-h. reflux with 200 mL. concentrated HCl and 100 mL. EtOH yielded 2,4,6-HOMe2C6H2CH2NH2.HCl, m. 160° (decomposition) (AcOH), condensed with 2,4,6-HOMe2C6H2CHO (XII) in the presence of NaHCO3 to 2,4,6-HOMe2C6H2CH2N:CHC6H2Me2OH-4,6,2 (XIII), m. 203°; reduction over Pt gave VII. A mixture of 2 g. [2,3,5-HOMe2C6H2CH2]2NH (XIV), 6.2 g. m-O2NC6H4SO3Na (XV), and 3 g. NaOH in 10 mL. H2O boiled 2 h., acidified with H2SO4, and steam-distilled (method A) gave 1.10 g. 2,3,5-HOMe2C6H2CHO (XVI), m. 26° [oxime, m. 139° (petr. ether)], and 0.4 g. 2,3,5-HOMe2C6H2CO2H, m. 179°; 2 g. XIV, 6 g. XV, and 30 mL. AcOH refluxed 2 h. formed 1.6 g. XVI (method B); [2,3,5-HO(Cl)2C6H2CH2]2NH treated by A gave 55% 2,3,5-HOCl2C6H2CHO (XVII), m. 95° (oxime, m. 196°), and some 2,3,5-HOCl2C6H2CO2H, m. 224°, IV formed by A 36% 5,2,3,6-Br(OH)Me2C6HCHO (XVIII), m. 87° (oxime, m. 181°), and some 5,2,3,6-Br(OH)Me2C6HCO2H, m. 239°; XVIII was obtained in 75% yield by B; III yielded 27% 5,2,3,6-Cl(OH)(Me2CH)MeC6HCHO (XIX), m. 59° (oxime m. 164°), by A, 71% by B; [4,3,5-HOMe2C6H2CH2]3N yielded by A 25% 4,3,5-HOMe2C6H2CHO, m. 115° (oxime, m. 190°), and some (4,3,5-HOMe2C6H2)2CO, m. 215°; VI gave 33% 2,5-HOMeC6H3CHO, m. 56°, by A, none by B; [2,5-HO(tert-Bu)C6H3CH2]3N gave 29% 2,5-HO(tert-Bu)C6H3CHO (XX) (oxime m. 113°) and some 2,5-HO(tert-Bu) C6H3CO2H, m. 151°, by A, nothing by B; VIII yielded 10% 2,3,6-HOMe2C6H2CHO by A, while VII formed only traces of an aldehyde; 2,6,3-[2,5-HO(tert-Bu)C6H3CH2NHCH2]2(tert-Bu)C6H2OH gave by A XX and 2,6,4-(CHO)2(tert-Bu)C6H2OH, m. 106° (oxime m. 113°); XI and XIII yielded by A XVI and XII, resp. A mixture of 5 g. 2,4-xylenol and 16.5 g. II heated 3 h. at 140°, treated with 15 g. XV in 60 mL. AcOH, boiled 2 h., and steam-distilled gave 4.1 g. XVI; similarly, p-chlorothymol formed 78% XIX; 4,2,6-Br-Me2C6H2OH gave 75% XVIII; treatment of 2,4-Cl2C6H3OH with II, followed by reflux

with NaOH and XV gave 55% XVII.

IT 75551-86-9P, Phenol, 2-(aminomethyl)-3,5-dimethyl-, hydrochloride
99985-48-5P, Acetamide, N-(4,6-dimethylsalicyl)-
100129-50-8P, Acetamide, N-(5-chloro-4,6-dimethylsalicyl)-
109247-43-0P, Phenol, 2,2'-(iminodimethylene)bis[3,5-dimethyl-
RL: PREP (Preparation)
(preparation of)

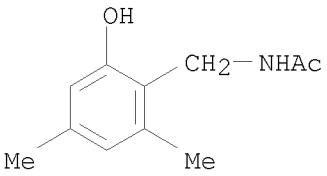
RN 75551-86-9 CAPLUS

CN Phenol, 2-(aminomethyl)-3,5-dimethyl-, hydrochloride (6CI, 9CI) (CA INDEX NAME)



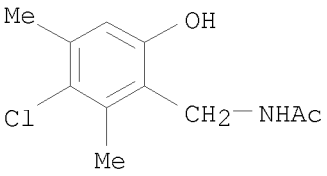
RN 99985-48-5 CAPLUS

CN Acetamide, N-(4,6-dimethylsalicyl)- (6CI) (CA INDEX NAME)



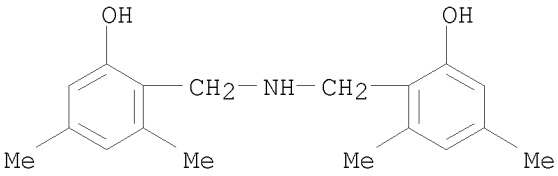
RN 100129-50-8 CAPLUS

CN Acetamide, N-(5-chloro-4,6-dimethylsalicyl)- (6CI) (CA INDEX NAME)



RN 109247-43-0 CAPLUS

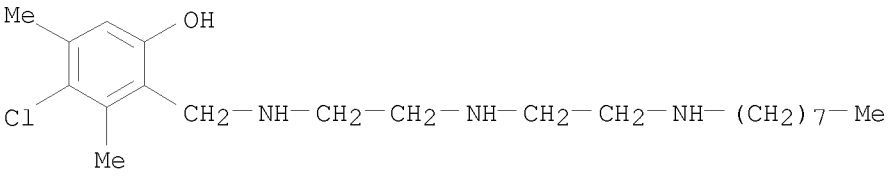
CN Phenol, 2,2'-(iminodimethylene)bis[3,5-dimethyl- (6CI) (CA INDEX NAME)



L4 ANSWER 25 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1960:59461 CAPLUS
DN 54:59461
OREF 54:11521c-e
TI Amphoteric surface-active organic compounds
IN Schmitz, Adolf; Cramer, Gunter
PA Goldschmidt Akt.-Ges.
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2907791		19591006	US 1955-508768	19550516

AB These compds. possessing germicidal and detergent properties may be prepared by causing to react at elevated temps. an amine, HCHO, and a phenol. Thus, PhOH 94, dodecyldiethylenetriamine (I) 271, and 37% HCHO 81 parts were caused to react with considerable heat evolution. A light yellow sirup, 1-dodecyl-7-(x-hydroxybenzyl)diethylenetriamine, resulted. Similarly treated were: p-chloro-m-cresol, I, and HCHO; p-cresol, octyldiethylenetriamine (II), and HCHO; p-chloro-m-xylenol, II, and HCHO; phenol, 4-dodecylbenzyltriethylenetetramine, and HCHO; p-cresol, II (2 moles), and HCHO (2 moles); p-chloro-m-cresol, I (2 moles), and HCHO (2 moles); salicylic acid, I (2 moles), and HCHO (2 moles); p-hydroxybenzoic acid, I (2 moles), and HCHO (2 moles); 2,2-bis(4-hydroxyphenyl)propane, I (4 moles), and HCHO (4 moles). The salicylic acid derivative kills Micrococcus aureus (Staphylococcus aureus), Escherichia coli, and Bacterium proteus vulgaris (Proteus vulgaris) in a 1:8000 dilution in 10 min.
IT 103508-55-0, Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]-
(amphoteric germicidal surface-active)
RN 103508-55-0 CAPLUS
CN Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (6CI) (CA INDEX NAME)



L4 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1960:22796 CAPLUS
DN 54:22796
OREF 54:4442f-i,4443a-h
TI The structure of artificial rosins. VII. Oxidative degradation of the methylene-nitrogen bridges in phenol-hexamethylenetetramine condensates
AU Zigeuner, G.; Jellinek, K.
CS Univ. Graz, Austria
SO Monatshefte fuer Chemie (1959), 90, 232-8
CODEN: MOCMB7; ISSN: 0026-9247
DT Journal
LA Unavailable
AB cf. C.A. 53, 15000h. Degradation via oxidative alkali melts gives insight

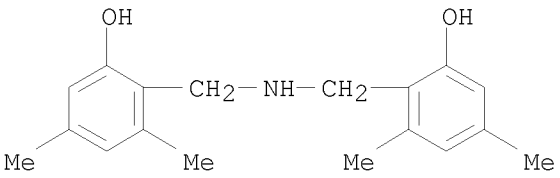
into the hardening of PhOH with (CH2)6N4, e.g. bonding occurs mainly in the o-position of PhOH with formation of dibenzylamines and chains, while bonding in the p-position occurs only after prolonged heating and higher temps. 2,2'-Dihydroxy-3,3',5,5'-tetramethyldibenzylamine (I) and tris(2-hydroxy-3,5-dimethylbenzyl)amine (II) are easily converted to hydroxytrimesic acid (III) by use of an oxidative alkali melt with PbO2 which rapidly degrades the CH2-N bridges, but under the same conditions 2,2'-dihydroxy-3,3',6,6'-tetramethylbenzylamine (IV) and 2,2'-dihydroxy-4,4',6,6'-tetramethylbenzylamine (V) undergo decarboxylation, IV to 2-hydroxyisophthalic acid (VI), and V to 2-hydroxyterephthalic acid (VII) and 5-hydroxyisophthalic acid (VIII). The degradation of xylenol-(CH2)6N4 condensates IV and V via oxidative alkali melts proceeds along unknown paths and leads to products from whose constitution the structure of the starting materials cannot be determined with certainty, but the degradation of PhOH-(CH2)6N4 condensates proceeds without side reaction, e.g. o-hydroxybenzylamine (IX) and 2,2'-dihydroxydibenzylamine (X) form salicylic acid (XI), 4-hydroxybenzylamine, 4,4'-dihydroxydibenzylamine, and the tribenzylamine (XII) yield p-hydroxybenzoic acid (XIII). The three-ring compds. 2,6-bis(2-hydroxybenzylaminomethyl)phenol (XIV) and 2,6-bis(4-hydroxybenzylaminomethyl)phenol (XV) are synthesized by dehalogenation of 2,6-bis(acetylaminomethyl)-4-chlorophenol (XVI) with Raney Ni to 2,6-bis(acetylaminomethyl)phenol (XVII), saponification of XVII to 2,6-bis(aminomethyl)phenol (XVIII), which with o-, and p-HOC6H4CHO, resp., forms the three-ring azomethine from which is formed XIV and XV by catalytic hydrogenation. Via oxidative alkali melts XIV is split into XI and VI, and XV into XI and VI. The separation of the acids is worked out preparatively, also the paper chromatography of the phenol carboxylic acids. The PhOH-(CH2)6N4 rosins are prepared by hardening PhOH and (CH2)6N4 in 3:2 mole ratio at various temps, and reaction times. PhOH and (CH2)6N4, on hardening at 100°, combine almost exclusively in the o-position with the formation of X and o-substituted chains of the type XIV. Only on oxidative degradation of rosins which are hardened longer at 100° and above can the formation of XVII be observed, which supposes the formation of p-compds. But here too, the o-compds. XI and VI constitute the main yield. Hardening at 180° of a condensate which forms at 100° by a three-dimensional bonding with NH3 splitting off forms III through oxidative degradation. Through oxidative degradation are affected not only CH2-N bridges, but also CH2 bridges. The PhOH-(CH2)6N4 condensates obtained at 100-30° contain mainly CH2-N bridges, as shown by N values, while those obtained at 180° contain CH2 bridges besides, although the position of the bridges cannot be determined by the results. PhOH-(CH2)6N4 condensate (2 g.) is mixed intimately with 9-11 g. PbO2 and introduced portionwise with good stirring into a melt of 40 g. KOH and 10 g. H2O at 320°, cooled, carefully diluted with 50 ml. H2O, acidified with 50% H2SO4, made alkaline, the precipitated PbSO4 separated and washed well, the filtrate acidified again, extracted several times with ether, the ether dried, evaporated, and the residue treated with superheated steam to yield XI. The residue is extracted with hot H2O, VI crystallizing out of the filtrate. The residue contains XII. III is obtained by evaporating the aqueous phase after Et2O separation and extraction of the evaporated residue. Oxidation of I yields 76% III and of II, 75% III. Yields of VI from IV and VII and VIII from V are small. On paper chromatography the following results are obtained with S & S 2043a/gl, descending in 80:4:16 EtOH-concentrated aqueous NH3-H2O, 1% FeCl3 solution as developer (acid, RF, color of spots, and

ultraviolet fluorescence given): XI, 0.75, blue, strongly blue; XIII, 0.57, weakly yellow, -; VII, 0.50, blue, strongly light blue; 4-hydroxyphthalic acid, 0.41, violet, weakly blue; VI, 0.31, pink, dark blue; VIII, 0.25, -, strongly yellow; III, 0.12, yellow-brown, blue. p-ClC6H4OH (60 g.) is dissolved in 150 ml. saturated alc. HCl and treated with methylolacetamide (from 70 g. AcNH2 and 35 g. paraformaldehyde), HCl gas added 24 hrs. under ice cooling, the precipitating XVI.HCl separated, taken up in H2O, and XVI liberated by dilute NH3 in 60% yield, m. 202° (40% EtOH). XVI (6 g.) in 100 ml. EtOH, 3 ml. H2O and 0.9 g. NaOH is hydrogenated in the presence of 10 g. Raney Ni till H absorption ceases, neutralized, the solvent evaporated in vacuo, and the residue recrystd. from H2O several times to yield XVII, prisms, m. 175°, yield 80%. Over 30 g. XVII is poured 50 ml. EtOH and 150 ml. HCl (d. 1.19), and with addition of HCl 6-8 hrs. refluxed, cooled, and saturated with HCl gas to precipitate XVIII.HCl, long spears, m. 215° (decomposition). XVIII.HCl (11.5 g.) is dissolved in 100 ml. EtOH, and boiled 30 min. with 12.5 g. o-HOC6H4CHO and 8.6 g. NaHCO3. On cooling, the azomethine (XIX), yellow needles, m. 187° (xylene), seps. XIX (2 g.) is dissolved in 50 ml. EtOH and 3 ml. HCl (d. 1.19) and hydrogenated with a PtO2 slurry (100 mg. PtO2 in 20 ml. EtOH). Evaporation yields hygroscopic crystals of XIV.HCl, from which is obtained XIV (decomposition from 180°) through NaHCO3 treatment. In the same manner XV is obtained by treatment of XVIII with p-HOC6H4CHO and NaHCO3 to form the azomethine, weakly yellow needles, m. 183°, which is then reduced to XV.HCl, hygroscopic needles, and XV, decompose from 160°, liberated by NaHCO3 treatment.

IT 109247-43-0P, Phenol, 2,2'-(iminodimethylene)bis[3,5-dimethyl-
RL: PREP (Preparation)
(preparation of)

RN 109247-43-0 CAPLUS

CN Phenol, 2,2'-(iminodimethylene)bis[3,5-dimethyl- (6CI) (CA INDEX NAME)



L4 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1959:94827 CAPLUS

DN 53:94827

OREF 53:17141d-h

TI The substitution of Mannich groups on some halogenated phenols

AU Berger, Jerry E.; Byrd, David S., Jr.; Meadow, J. R.

CS Univ. of Kentucky, Lexington

SO Trans. Kentucky Acad. Sci. (1958), 19, 77-82

DT Journal

LA Unavailable

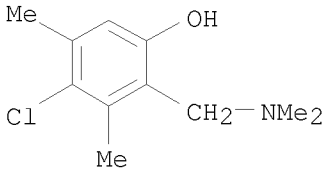
AB Mono- and di-Mannich bases of several halogenated phenols were prepared in 75-95% yields. A mixture of 9.36 g. 3,5-dimethyl-4-chlorophenol (I), 4.4 g. pyrrolidine, and 15 ml. absolute EtOH was cooled in ice and treated with 5.4 g. 37% HCHO to give 82.5% 2-(2-pyrrolidinyl)methyl-3,5-dimethyl-4-chlorophenol, m. 44-5° (EtOH), which with HCHO and pyrrolidine gave

88.8% 2,6-bis(2-pyrrolidinyl)methyl-3,5-dimethyl-4-chlorophenol, m. 103.5-4.5°. In similar reactions of other halogenated phenols and secondary amines with HCHO the following Mannich bases were prepared (phenol, Mannich substituent group ortho to the OH, and m.p. given): 6-chlorothymol (II), Me2NCH2, 54.5-5.5°; II, Et2NCH2, 26-7°; II, morpholinomethyl, 88-9°; II, N-methylpiperazinomethyl, 87-7.5°; II, piperidinomethyl, 85-6.5°; II, 1-pyrrolidinylmethyl, 58-9°; I, 2-Me2NCH2, 63-4°; I, 2,6-(Me2NCH2)2, 41-3° (probably a mixture); I, 2-morpholinomethyl, 127-8°; I, 2,6-dimorpholinomethyl, 174-6°; I, 4-methyl-1-piperazinylmethyl, 132-2.5°; I, piperidinomethyl, 148.5-9°; 4-bromophenol, piperidinomethyl, 60-2.5°; 4-bromophenol, 1-pyrrolidinylmethyl, 75-6°; 4-chlorophenol, 1-pyrrolidinylmethyl, 69-71°; 2,4-dichlorophenol (III), Me2NCH2, 60.5-1.5°; III, morpholinomethyl, 91.5-2°; III, piperidinomethyl, 80.5-1°; III, 1-pyrrolidinylmethyl, 46.5-7.5°; 2,4,5-trichlorophenol (IV), Et2NCH2, 81-2.5°; IV, morpholinomethyl, 138.5-9.5°; IV, 4-methyl-1-piperazinomethyl, 88-9°; IV, piperidinomethyl, 110-11.5°; IV, 1-pyrrolidinylmethyl, 80-2°

IT 99980-84-4P, Phenol, 4-chloro-2-(dimethylaminomethyl)-3,5-dimethyl-
RL: PREP (Preparation)
(preparation of)

RN 99980-84-4 CAPLUS

CN Phenol, 4-chloro-2-(dimethylaminomethyl)-3,5-dimethyl- (6CI) (CA INDEX NAME)



L4 ANSWER 28 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1958:55740 CAPLUS

DN 52:55740

OREF 52:9992b-g

TI Series of ω-dimethylaminoalkylphenols

AU Brown, J. P.; McCall, E. B.

CS Monsanto Chem. Ltd., Wrexham, N. Wales

SO Journal of the Chemical Society (1957) 3875-80
CODEN: JCSOA9; ISSN: 0368-1769

DT Journal

LA Unavailable

OS CASREACT 52:55740

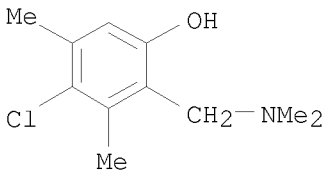
AB 4,3,5-ClMe2C6H2OH (I) with aqueous CH2O and Me2NH gave 4,3,5,2-ClMe2(Me2NCH2)C6HOH (II), m. 65-6° (MeOH). 4,3,5-ClMe2C6H2OMe (III), CH2O, and 32% HCl gave 4,3,5,2-ClMe2(ClCH2)C6HOMe (IV), m. 91-2°. IV and NaCN gave the cyanide, m. 120-22°, which was hydrolyzed to 4,3,5,2-ClMe2(HO2CCH2)C6HOMe, m. 164-6°. This with SOCl2 and then Me2NH gave the N,N-dimethylamide, m. 130-1°, reduced by LiAlH4 to 4,3,5,2-ClMe2(Me2NCH2CH2)C6HOH (V), m. 130-2°. Similarly prepared (m.ps. given) were 4,3,5,2-ClMe2[Me2N(CH2)3]C6HOH (VI), 100-2°, from the N,N-dimethylamide, 104-5°, of

4,3,5,2-ClMe2(HO2CCH2CH2)C6HOMe (VII), 116-17°, and 4,3,5,2-ClMe2[Me2N(CH2)4]C6HOH (VIII), 159-60°, from the N,N-dimethylamide, 83-6°, of 4,3,5,2-ClMe2[HO2C(CH2)3]C6HOMe (IX), 117-18°. VII was obtained by malonic ester synthesis from IV; 2,3,5,4-ClMe2[(HO2C)2CHCH2]C6HOMe m. 166-8°; di-Et ester, m. 77-8°. IX resulted from Clemmensen reduction of 4,3,5,2-ClMe2[HO2C(CH2)2CO]C6HOMe, m. 178-81°, prepared from III, (CH2CO)2O, and AlCl3. I and ClCH2COCl (X) gave the chloroacetate, m. 50-2°, which on heating with AlCl3 cyclized to 5-chloro-4,6-dimethylcoumaranone, m. 137-40°. Similarly I and Cl(CH2)2COCl gave the β-chloropropionate, m. 51-2°, which cyclized to 6-chloro-5,7-dimethylchromanone, m. 70-1° (2,4-dinitrophenylhydrazone m. 265°), identical with the product prepared by H2SO4 treatment of 4,3,5-ClMe2C6H2O(CH2)2CO2Et (XI), m. 46-9°. XI resulted from the reaction of CH2:CHCO2Et with I in the presence of the Na salt of I. III, X, and AlCl3 gave 4,3,5,2-ClMe2(ClCH2CO)C6HOMe, m. 133-5°, converted with Me2NH to 4,3,5,2-ClMe2(Me2NCH2CO)C6HOMe; hydrochloride m. 210-25°. An attempted azlactone synthesis from 4,3,5,2-ClMe2(HCO)C6HOH gave 3-acetamido-6-chloro-5,7-dimethylcoumarin, subliming above 300°. III, HCONMePh, and POCl3 gave a little 4,3,5,2-ClMe2(HCO)C6HOMe, m. 106-7°. Also prepared were (m.ps. given): the OH analog (XII), 145-50°, of IX; the dimethylamide, 182-3°, of XII, which with LiAlH4 gave VIII; 3,5,2-Me2[HO2C(CH2)3]C6H2OH (XIII), 130-32°, from IX with 66% HI; the dimethylamide, 179-81°, of XIII; the Me ester (XIV), 41°, of IX; 4,3,5,2-ClMe2[HO(CH2)4]C6HOMe (XV), 61°, from XIV with LiAlH4; p-nitrobenzoate, 89-91°, of XV; 4,3,5,2-ClMe2[Br(CH2)4]3,5-Me2C6HOMe, 124°, from XV and 48% HBr; quaternary salt,, 186-90°, from C5H5N.HCl and XV; 4,3,5,2-ClMe2[HO(CH2)4]C6HOH, 105-6°, from XII and LiAlH4. In vitro II, V, VI, VIII and their quaternary salts showed poor to moderate antibacterial activity, increasing with the length of the alkyl group, against Bacillus mycoides, Staphylococcus aureus, and Escherichia coli.

IT 99980-84-4P, Phenol, 4-chloro-2-(dimethylaminomethyl)-3,5-dimethyl-
RL: PREP (Preparation)
(preparation of)

RN 99980-84-4 CAPLUS

CN Phenol, 4-chloro-2-(dimethylaminomethyl)-3,5-dimethyl- (6CI) (CA INDEX NAME)



L4 ANSWER 29 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1957:69146 CAPLUS

DN 51:69146

OREF 51:12516h-i,12517a,12518a

TI Cleaning, foaming, and wetting agents

IN Hirschmann, Alexandre

PA Etablissements Fournier-Ferrier

DT Patent

LA Unavailable
FAN.CNT 1

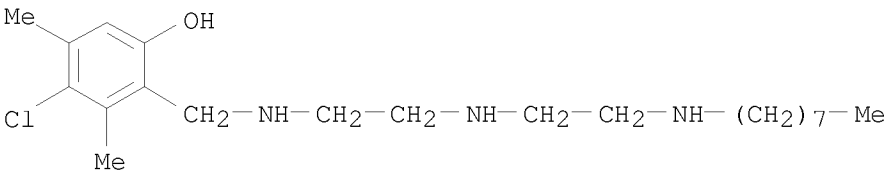
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1007215		19520505	FR	

AB Good wool-cleaning agents as well as wetting and foaming agents, containing in the same aromatic mol. an amide linkage and a polyoxyethylene group of the general formula RCOHNR'ArR''(OCH2CH2)nOH, where R is a fatty-acid radical, R' and R'' are aliphatic chains, Ar is a substituted mono- or polynuclear aromatic compound, and n is 4-16 or more, are prepared by condensation of at least 3 moles ethylene oxide with fatty amides, derived from >C6 fatty acids and from aromatic hydroxy-containing amines. These amides are represented by the general formula RCONHR'ArR''OH, RCONHArR''OH, RCONHR'ArOH, and RCONHArOH. Acid chlorides, prepared by the action of PCl3 on coconut-oil fatty acids (I), are condensed with p-aminophenol at 60-80°. The product thus obtained is condensed with 8-12 moles of ethylene oxide, giving products of the general formula RCONHC6H4(OCH2CH2)nOH, where n = 8-12. Oleic acid is condensed with p-aminobenzyl alc. and the reaction product is condensed with 12-16 moles of ethylene oxide to give the p-(methylenepolyglycolether)-oleylanilide. By condensation of I with p-aminophenylethyl alc. and 12-15 moles ethylene oxide, a product of the general formula RCONHC6H4CH2CH2(OCH2CH2)nOH is obtained.

IT 103508-55-0
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 103508-55-0 CAPLUS

CN Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (6CI) (CA INDEX NAME)



L4 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1957:69145 CAPLUS
DN 51:69145
OREF 51:12516g-h
TI Soap compositions
IN Aylesworth, Robert D.
PA Emery Industries, Inc.
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2792348		19570514	US 1952-316067	19521021

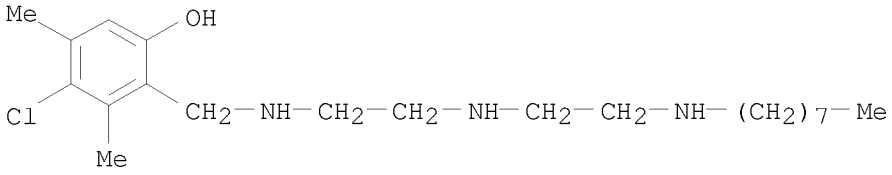
AB The drying of soaps is simplified if 0.1% of Na salts of dibasic acids (I) is included with ordinary fatty-acid soaps during manufacture This permits preparation of soaps of low-titer fatty acids without drying to abnormally low H2O content; preparation of solid soaps with a higher H2O content than normal when employing fatty acids of normal titer, such as tallow or cottonseed acids; and preparation of soap flakes or powders which, for a given H2O

content, are less friable and have less tendency to powder than normal products. The I include malonic, succinic, adipic, azelaic, and sebacic acids.

IT 103508-55-0
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 103508-55-0 CAPLUS

CN Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (6CI) (CA INDEX NAME)



L4 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1957:69141 CAPLUS

DN 51:69141

OREF 51:12515h-i,12516a-b

TI Amphoteric germicidal detergents

PA Th. Goldschmidt A.-G.

DT Patent

LA Unavailable

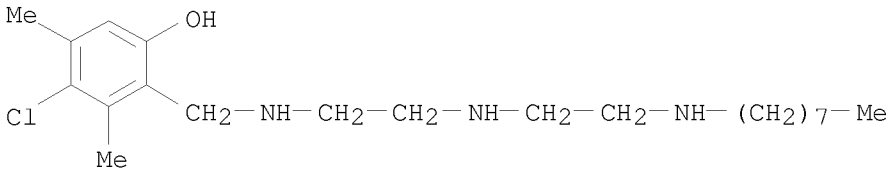
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI GB 771635		19570403	GB	
DE 1070189			DE	

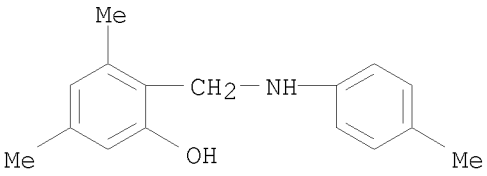
AB Compds. having high-bactericidal efficacy, as well as good wetting and detergency, are prepared by treating certain amines with HCHO and phenols. The general formula is: C6H(5-x-y)(RACH2)x(R')yOH, where x = 1-3 and y = 0-3, but x + y is not greater than 5, R is an alkyl or alkylaryl group having 8-18 C atoms, R' is an alkyl group with 1-3 C atoms, halogen, carboxyl, or C6H2(RACH2)2(OH)C(CH3)2-, and A is an amino group such as -NR''-, -NR''(C2H4NH)z-, -NR''(C3H6NH)z-, or where R'' is H or an alkyl group with 8-18 C atoms and z = 1-3. For example, octylamine 25.8, PhOH 1.8, and HCHO 6.0 parts were mixed and, after the exothermic reaction had subsided, the mixture was stirred for 1 hr. at 100°. After cooling, o- and p-(octylaminomethyl)phenol as light-yellow oil was obtained which dissolved to a colloidal solution in alkalies, and to a clear solution in dilute acids. Analogously, o- and p-(dodecyldiethylenetriaminomethyl)phenyl, 2-(dodecyldiethylenetriaminomethyl)-4-chloro-m-cresol, o-(octyldiethylenetriaminomethyl)-p-cresol, 2-(octyldiethylenetriaminomethyl)-4-chloro-m-xylenol, o- or p-[p-(dodecylbenzyl)triethylenetetraaminomethyl]phenol, 2,4- or 2,6-bis(tetradecylaminomethyl)phenol, 2,6-bis(octyldidiethylenetriaminomethyl)-p-cresol, 2,6-bis(dodecyldiethylenetriaminoethyl)-4-chloro-m-cresol, 3,5-bis(dodecyldiethylenetriaminomethyl)salicylic acid, 2,6-bis(dodecyldiethylenetriaminomethyl)-4-hydroxybenzoic acid, and 2,2-bis[4-hydroxy-3,5-bis(dodecyldiethylenetriaminomethyl)phenyl]propane were prepared

IT 103508-55-0P, Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]-

RL: PREP (Preparation)
(preparation of)
RN 103508-55-0 CAPLUS
CN Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (6CI) (CA INDEX NAME)



L4 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1956:12096 CAPLUS
DN 50:12096
OREF 50:2468b-e
TI The structure of artificial resins. II. The action of aromatic amines on dibenzylamines, tribenzylamines, and dibenzyl ethers
AU Zigeuner, G.; Weichsel, H.
CS Univ. Graz, Austria
SO Monatshefte fuer Chemie (1955), 86, 154-64
CODEN: MOCMB7; ISSN: 0026-9247
DT Journal
LA Unavailable
OS CASREACT 50:12096
AB cf. C.A. 48, 14285b. Cleavage with aromatic amines is employed for the degradation of phenol-(CH2)6N4 condensates and related model compds. R2NH[R = 2,3,5-HO(Me)2C6H2CH2] (I) (0.5 g.), and 1 g. urea, heated 3 h. at 160° gives a 95% yield RNHCONH2 (II), m. 192°. Treated similarly, R2N (III) gives 55% of II. I (0.5 g.) and 1 g. PhNH2, heated 2 h. at 160°, gives a 67% yield of PhNHR, m. 87°. Similarly, I and p-MeC6H4NH2 (IV) gives 63% of RNHC6H4Me-p (V), m. 98°. III and IV yield 55% of V. R2O (VI) (0.5 g.), heated with 1.5 g. urea for 2 h. at 160°, gives a 74% yield of II. VI (0.5 g.) and 1 g. IV heated 1 1/2 h. at 160° gives 73% of V. Other compds. similarly prepared were: 2,3-HO(Me)C6H3CH2NHC6H4Me-4, m. 76°; 2,3,6-HO(Me)2C6H2CH2NHC6H4Me-4, m. 143°; 2,4,6-HO(Me)2C6H2CH2NHC6H4Me-4, m. 125°; 2,5-HO(Me3C)C6H3CH2NHC6H4Me-4, m. 85°; 2,6-bis(p-toluidinomethyl)-4-methylphenol, m. 118°; 2,6-bis(p-toluidinomethyl)-3,5-dimethylphenol, m. 134°; 2,6-bis(p-toluidinomethyl)-4-tert-butylphenol, m. 108.5; 2,4,6-tris(2-hydroxy-3,5-dimethylbenzyl)-3,5-dimethylphenol, m. 209°; N-(4-hydroxy-3,5-dimethylbenzyl)anthranilic acid, m. 173° (Me ester, m. 115°); N-(4-hydroxy-2,5-dimethylbenzyl)anthranilic acid, m. 186°; N-(2-hydroxy-3,5-dimethylbenzyl)anthranilic acid, m. 165°.
IT 855410-04-7P, Phenol, 3,5-dimethyl-2-p-toluidinomethyl-
RL: PREP (Preparation)
(preparation of)
RN 855410-04-7 CAPLUS
CN Phenol, 3,5-dimethyl-2-[[(4-methylphenyl)amino]methyl]- (CA INDEX NAME)

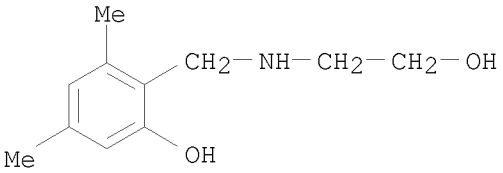


L4 ANSWER 33 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1955:75852 CAPLUS
DN 49:75852
OREF 49:14359e-i,14360a-b
TI The synthesis of amphoteric tanning materials. II,III
AU Rosenbusch, K.
CS Tech. Hochschule, Darmstadt, Germany
SO Leder (1955), 6, 80-6
CODEN: LEDEA8; ISSN: 0024-0176
DT Journal
LA Unavailable
AB Aliphatic amines, although more basic than aromatic amines, did not condense with monohydric phenols to amphotans in aqueous solution, but did in organic solvents. In MeOH, equimolar amts. of PhOH, dimethylamine, and HCHO condensed to an acid-soluble oil that was only partly soluble in alkali. The oil was separated to 2 fractions by Et2O-alkali extraction The main (alkali-insol.) fraction distilled without decomposition at 105-6° under 15 mm. pressure. It was identified as 2-hydroxy-N,N-dimethylbenzylamine by catalytic hydrogenation which gave a quant. yield of 1-methyl-2-cyclohexanol, which formed a 3,5-dinitrobenzoyl ester, m. 97°. It was not a tanning agent because the mol. was too small. Phenolnovolak condensed with dimethylamine in MeOH, to give an amphotan that was soluble in dilute acid and alkali and precipitated at the isoelec. point. The N content of 9% showed that one dimethylamine group had coupled with each phenolic group. The resin in acid form did not precipitate with gelatin until neutralized to the quaternary ammonium base stage. The cheaper ethanolamines also condensed with phenolnovolak; the mono compound giving a yellow alc.-insol. resin and the di-compound a resin soluble in alc., acid, or alkali. Catalytic hydrogenation of these resins produced p-cresol-novolak which was readily soluble in alc. or alkali but not in acid. The above condensations occur only in organic solvents, but polyhydric phenols form amphotans in aqueous solns. Diethanolamine condensed with HCHO to 3-(2-hydroxyethyl)oxazolidine, C5H11O2N, which distilled without decomposition at 128°, 31 mm., decomposed at b.p. 224° and formed a picrate m. 108°. It condensed with resorcinol to N,N-bis(2-hydroxyethyl)-2,4-dihydroxybenzylamine (hydrochloride, colorless needles, m. 145° with decomposition) and with pyrogallol to N,N-bis(2-hydroxyethyl)-3,4,5-trihydroxybenzylamine, m. 145°. These crystalline Mannich bases showed the typical behavior of amphotans. If the precipitate at the isoelec. point was filtered off, its N content approached that of a pure polyhydroxynovolak. Inorg. bases could also be used. NH4Cl, resorcinol, and HCHO, condensed to a tannin that penetrated rapidly because of its small mol. Mannich condensation could also be obtained by fusion. With monohydric phenols the products were soluble, whereas if condensed in aqueous solution they were insol. Sym-xylenol, HCHO, and monoethanolamine condensed to the mono-, di-, or tri-benzylamine

derivative, depending on the amount of amine used. Fusion of phenolnovolak, ethanolamine, and HCHO produced an amphotan similar to that made in alc. solution Condensation by fusion can also be obtained with polyhydric phenols and amine salts instead of the free base, provided free acid is absent. The most important use for the Mannich condensation in the tanning chemistry lies in the possibility of changing vegetable tannins to amphotannins. A type reaction for a hydrolyzable and a condensed tannin are shown. Exptl. work was reported previously (C.A. 48, 13249e).

IT 856374-44-2P, Ethanol, 2-(4,6-dimethylsalicylamino)-
856374-45-3P, Ethanol, 2-(4,6-dimethylsalicylamino)-, picrate
RL: PREP (Preparation)
(preparation of)

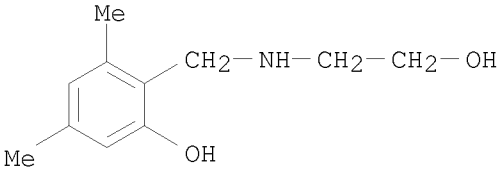
RN 856374-44-2 CAPLUS
CN Phenol, 2-[[(2-hydroxyethyl)amino]methyl]-3,5-dimethyl- (CA INDEX NAME)



RN 856374-45-3 CAPLUS
CN Ethanol, 2-(4,6-dimethylsalicylamino)-, picrate (5CI) (CA INDEX NAME)

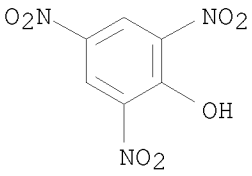
CM 1

CRN 856374-44-2
CMF C11 H17 N O2



CM 2

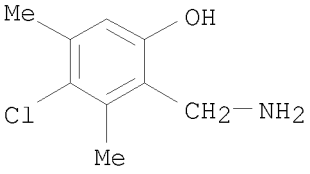
CRN 88-89-1
CMF C6 H3 N3 O7



L4 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

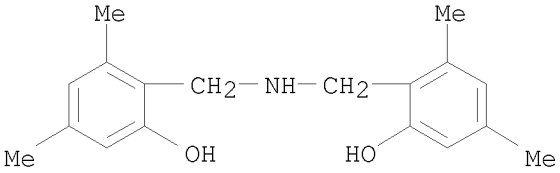
AN 1952:11359 CAPLUS
DN 46:11359
OREF 46:2009a-f
TI Method for preparing secondary amines and Schiff bases from phenols and hexamine
AU Duff, J. C.; Furness, V. I.
CS Coll. Technol., Birmingham, UK
SO Journal of the Chemical Society (1951) 1512-15
CODEN: JCSOA9; ISSN: 0368-1769
DT Journal
LA Unavailable
OS CASREACT 46:11359
AB The phenol (10 g.) and 4 g. H3BO3 in 40 mL. EtOCH2CH2OH, treated with 5 g. (CH2)6N4, refluxed 2 h., and poured into H2O, give the following amines; the yield is indicated. Bis(o-hydroxybenzyl)amine, m. 190-200° (decomposition), 2.5 g.; HCl salt; bis(2-hydroxy-3-methylbenzyl)amine, m. 150-5° (decomposition), 5.1 g.; 4-Me isomer, m. 150-7° (decomposition), 7.5 g.; 5-Me isomer, m. 168-70° (decomposition), 7.7 g.; HCl salt. Bis(2-hydroxy-5-chlorobenzyl)amine, m. 155-60°, 2.8 g.; HCl salt. Bis(2-hydroxy-5-chloro-6-methylbenzyl)amine, m. 185-90° (decomposition), 5.5 g.; HCl salt. Bis(2-hydroxy-1-naphthylmethyl)amine, m. 170-8° (decomposition), 6.1 g.; HCl salt. Bis(3-chloro-6-hydroxy-2,4-dimethylbenzyl)amine, m. 219° (decomposition), 6.8 g.; HCl salt. Bis(2-hydroxy-4, 6-dimethylbenzyl)amine, HCl, m. 215-20° (decomposition), 4.5 g. Bis(4-hydroxy-1-naphthylmethyl)amine, pale yellow, m. 205° (decomposition), 4.7 g.; HCl salt. The above amines are not hydrolyzed on boiling in EtOH with HCl. Schiff bases were obtained on heating 5 g. amine and 5 g. (CH2)6N4 in 15 mL. AcOH on the water bath (time and yield given). 2-Hydroxy-N-(2-hydroxybenzylidene)benzylamine (16 h.), bright yellow, 1.2 g.; 2-hydroxy-N-(2-hydroxy-3-methylbenzylidene)-3-methylbenzylamine (9 h.), orange, 3.8 g.; 2-hydroxy-N-(2-hydroxy-4-methylbenzylidene)-4-methylbenzylamine (9 h.), bright yellow, 2.7 g.; 2-hydroxy-N-(2-hydroxy-5-methylbenzylidene)-5-methylbenzylamine (9 h.), bright yellow, 3.5 g.; 5-chloro-2-hydroxy-N-(5-chloro-2-hydroxybenzylidene)benzylamine (6 h.), yellow, 4.2 g.; 3-chloro-6-hydroxy-N-(3-chloro-6-hydroxy-2-methylbenzylidene)-2-methylbenzylamine (6 h.), bright yellow, 3.7 g.; 3-chloro-N-(3-chloro-6-hydroxy- 2,4- dimethylbenzylidene)-6-hydroxy-2,4-dimethylbenzylamine (6 h.), orange yellow, 3.7 g.; 2-hydroxy-N-(2-hydroxy-5-phenylbenzylidene)-5-phenylbenzylamine (6 h.), bright yellow, 4.9 g.; 2-hydroxy-N-(2-hydroxy-4,6-dimethylbenzylidene)-4,6-dimethylbenzylamine (2 h.), bright yellow, 2 g.; 4-hydroxy-N-(4-hydroxy-1-naphthylmethylene)-1-naphthylmethylamine (2 h.), yellow, 4.3 g. Hydrolysis of the Schiff bases was carried out by heating 2 g. in 20 mL. of a mixture of equal vols. of EtOH and HCl (d. 1.17) to the b.p. and steam distilling the filtrate. The products are the corresponding aldehyde, the amine, and NH4Cl. 4-Chloro-2-formyl-3-methylphenol, m. 100.5°; 3-chloro-6-hydroxy-2,4-dimethylbenzylamine-H Cl. (PhCH2)2NH (5 g.) and 1 g. (CH2)6N4 in 11 mL. AcOH, boiled 5 min., give 1.2 g. BzH and PhCH2NH2. These reactions are regarded as explaining the mechanism of the general method for preparing o-hydroxyaldehydes described by Duff (C.A. 36, 1597.3).
IT 75552-02-2P, Phenol, 2-(aminomethyl)-4-chloro-3,5-dimethyl-, hydrochloride 859784-25-1P, 3,5-Xylenol, 2,2'-(iminodimethylene)di-, hydrochloride 859784-27-3P, 3,5-Xylenol, 2,2'-(iminodimethylene)bis[4-chloro-, hydrochloride 859784-30-8P, 3,5-Xylenol, 2,2'-(iminodimethylene)bis[4-chloro-
RL: PREP (Preparation)
(preparation of)

RN 75552-02-2 CAPLUS
CN Phenol, 2-(aminomethyl)-4-chloro-3,5-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



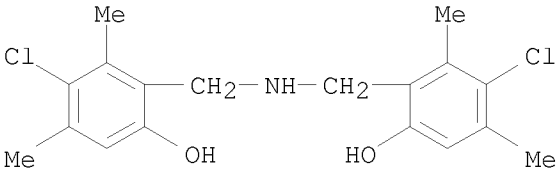
● HCl

RN 859784-25-1 CAPLUS
CN 3,5-Xylenol, 2,2'-(iminodimethylene)di-, hydrochloride (5CI) (CA INDEX NAME)



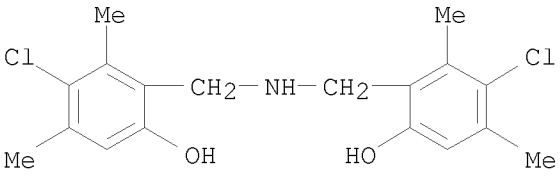
● HCl

RN 859784-27-3 CAPLUS
CN Phenol, 4-chloro-2-[[[(3-chloro-6-hydroxy-2,4-dimethylphenyl)methyl]amino]methyl]-3,5-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

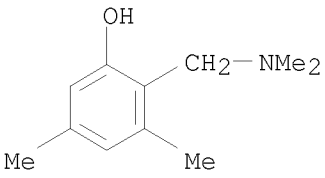


● HCl

RN 859784-30-8 CAPLUS
CN Phenol, 4-chloro-2-[[[(3-chloro-6-hydroxy-2,4-dimethylphenyl)methyl]amino]methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1951:49820 CAPLUS
DN 45:49820
OREF 45:8475d-f
TI Formaldehyde condensations with phenol and its homologs. XI. The preparation of 2-hydroxymethyl-3,5-dimethylphenol by a new general method
AU Finn, S. R.; Musty, J. W. G.
SO Journal of Applied Chemistry (1951), 1, 182-4
CODEN: JACHAU; ISSN: 0021-8871
DT Journal
LA Unavailable
AB cf. C.A. 45, 7074e. 3,5-Xylenol (I) with HCHO (II) forms substances other than 2-methylol-3,5-xylenol (III) (cf. C.A. 45, 1537). The diacetate (IV), b0.5 152-3°, n20D 1.5040°, of III resulted in 11 g. yield by refluxing 10 g. 2-(dimethylaminomethyl)-3,5-xylenol (V) 6 hrs. with 15 ml. Ac2O and also from III with Ac2O and K2CO3 but not with Ac2O and H2SO4. 2,4,6-Me2(HO)C6H2CHO (5.7 g.) in dry Et2O was added gradually to 1.1 g. LiAlH4 and Et2O, the mixture poured after 20 min. into cold H2O, allowed to stand 24 hrs. with addition of HOAc to maintain acidity, neutralized, filtered to remove inorg. solids, and the solution was concentrated in vacuo to 0.2 volume and cooled to give 1.67 g. solid, m. 60-6°. Recrystn. from petr. ether-C6H6 gave III, m. 88°. A similar reduction of IV (10.2 g.) with 3 g. LiAlH4 gave 1 g. III. The synthesis of III by way of V is according to the new general method (C.A. 45, 6168i). The phenylurethan of III m. 171°.
IT 63487-28-5P, Phenol, 2-(dimethylaminomethyl)-3,5-dimethyl-
RL: PREP (Preparation)
(preparation of)
RN 63487-28-5 CAPLUS
CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



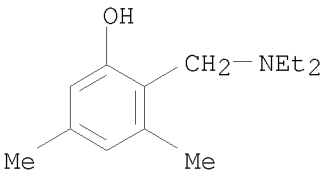
L4 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1947:2215 CAPLUS
DN 41:2215
OREF 41:414c-i,415a-i,416a-i
TI Aminoalkylphenols as antimalarials. I. Simply substituted α-aminocresols
AU Burckhalter, J. H.; Tendick, F. H.; Jones, Eldon M.; Holcomb, W. F.;

Rawlins, A. L.
CS Parke, Davis Co., Detroit, MI
SO Journal of the American Chemical Society (1946), 68, 1894-1901
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB In this paper Q-B4 indicates the quinine equivalent of the compound against P. gallinaceum in chicks, Q-D1 against P. lophurae in ducks, and Q-D2 and Q-J1 against P. cathemerium in ducks and canaries, resp. A value of 0.2 represents the activity of a drug that is 20% as effective as quinine; 0.2i indicates that the drug is inactive at 5 times the ED of quinine, and 0.2t indicates that at 0.2i the drug is toxic. The fact that 4,2-Me3CCH2CMe2(Me2NCH2)C6H3OH (I) (SN 5018) (U.S. 2,033,092, C.A. 30, 2669.2) was found to have Q-B4 0.3 and Q-J1 0.67i led to the synthesis of several hundred derivs. of o-H2NC6H4OH, of which 109 new compds. (and pharmacol. tests on 19 others) are reported in the present paper. The compds. were prepared by the Mannich reaction, in which phenols with at least one open position ortho or para to a phenolic HO group were treated with HCHO and aliphatic amines; (HCHO)3 and 37% HCHO were equally useful in the reaction. An equimol. mixture of the amine and HCHO in sufficient EtOH to give a clear solution on heating is added (after cooling) to the phenol in EtOH (solution or suspension), the mixture allowed to stand 1 h., refluxed 2 h., the solution concentrated, extracted with ether, and the substituted amine isolated as such or as the HCl(HBr) salt. Various modifications of this procedure are indicated. (AcCH2)2 (57 g.), 54.5 g. p-H2NC6H4OH, 100 cc. absolute EtOH, and 1 cc. AcOH, refluxed 20 h., give 82% 4-(2,5-dimethyl-1-pyrryl)phenol, m. 104-6° (not analyzed because of discoloration in air and light). (4-HOC6H4)2O (preparation in 40% yield given) (20.2 g.), 27.8 g. K2CO3, and 150 cc. Me2CO, heated to boiling, treated with 24.2 g. CH2:CHCH2Br during 30 min., the mixture refluxed 2 h., and the resulting allyl ether heated at 250°/20 mm., give 52% 3,3'-diallyl-4,4'-oxybiphenol, b1.5 195-200°. 2-Allyl-4-tert-butylphenol, b8 127-9°, 79%. The MeCl derivative of I (SN 7867) has Q-B4 0.3i. The following derivs. of 4-(1,1,3,3-tetramethylbutyl)-o-cresol were prepared: α-diamylamino (SN 7494), whose HBr salt m. 143°, 81%, Q-B4 0.05i; α-1-piperidyl (SN 6798), m. 70°, 95%, Q-B4 0.02; α-4-morpholinyl-HCl (SN 7137), m. 200°, 52%, Q-B4 0.03i; α-[ethyl(2-hydroxyethyl)amino]-HCl (SN 7821), m. 151°, 93%, Q-B4 0.08; α-[bis(2-hydroxyethyl)amino] (SN 6803), m. 81°, 24%, Q-B4 0.03; α-dibenzylamino (SN 6797), m. 118°, 70%, Q-B4 0.02i; 6-methyl-α-dimethylamino (SN 6804), Q-B4 0.20; 6-chloro-α-diethylamino (SN 7491), Q-B4 0.11. Derivs. of α-dimethylamino-o-cresol, (SN 7502), Q-B4 0.03i, prepared were: 6-Me (SN 7498), Q-B4 0.03i, Q-J1 0.05i; 4-tert-Bu (HCl salt) (SN 7497), Q-B4 0.1. α-Diethylamino-o-cresol (II) (SN 4769) b3 100-10° (HCl salt, m. 135°, 32%, Q-J1 0.2i). Derivs. of II: 6-Me, b3 107-8° (HCl salt, m. 161°, 36%, Q-B4 0.05t); 4-Me (SN 6805), b4 122, 71%, Q-B4 0.04 (HCl salt, m. 157°, Q-J1 0.05i); 4-tert-Bu (SN 7496), m. 36°, 38%, Q-B4 0.4; 4-tert-butyl-6-hydroxy (SN 7741), m. 142°, 96%, Q-B4 0.07i; 4-(2-methylcyclohexyl) (HCl salt) (SN 7503), m. 148°, 46%, Q-B4 0.18t; 6-heptyl (HCl salt) (SN 8459), m. 126°, 46%, Q-B4 0.1; 4-octyl (HCl salt) (SN 8458), m. 86°, 39%, Q-B4 0.04i; 4-dodecyl (SN 7500), Q-B4 0.10; 4-Cl (HCl salt) (SN 7493), m. 158°, 56%, Q-B4 0.06; 4-Br (HCl salt) (SN 7488), m. 165°, Q-B4 0.06; 6-Br (HCl salt) (SN 7296), m. 175°, 10%, Q-B4 0.05i; 4-methyl-6-bromo (HCl salt) (SN 13,700), m. 170°, 65%, Q-B4 0.05i; 4-bromo-6-Me (HCl salt) (SN 8456), m. 175°, 38%, Q-B4 0.4t; 6-cyclohexyl-6-bromo (SN

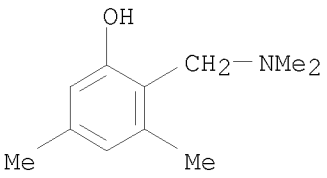
9000), m. 92°, 63%, Q-B4 0.06; 4-chloro-6-(3-buten-2-yl) (HCl salt) (SN 8294), m. 130°, 44%, Q-J1 1.0; 4-tert-amyl-6-chloro (HCl salt) (SN 7492), m. 148°, 83%, Q-B4 0.1; 4-chloro-5-Me (HCl salt) (SN 8497), m. 192°, 51%, Q-B4 0.08; 3-methyl-4-chloro-6-hexyl (HCl salt) (SN 8370), m. 132°, 81%, Q-B4 0.06; 4,5-di-Me (HCl salt) (SN 7304), m. 190°, 83%, Q-B4 0.2t; 3,5-di-Me (HCl salt) (SN 10,989), m. 156°, 77%, Q-B4 0.25; 3,5,6-tri-Me (HCl salt) (SN 7303), m. 175°, 94%, Q-B4 0.10, Q-J1 0.4t; 4-tert-butyl-5-Me (HCl salt) (SN 10,505), m. 177°, 12%, Q-B4 0.05i; 4-tert-butyl-6-Me (HCl salt) (SN 9576), m. 150°, 45%, Q-B4 0.3, Q-J1 1.0; 4-tert-butyl-6-allyl (HCl salt) (SN 7819), m. 139°, 48%, Q-B4 0.2; 4-tert-amyl-6-allyl (HCl salt) (SN 8051), m. 151°, 41%, Q-B4 0.17; 4-cyclohexyl-6-allyl (HCl salt) (SN 8383), m. 142°, 59%, Q-B4 0.18; 4-tert-butyl-6-cyclohexyl (HCl salt) (SN 8393), m. 192°, 56%, Q-B4 2.0. 4-Chloro-α-(1-piperidyl)-o-cresol (SN 6799) m. 57°, 82%, Q-B4 0.04i; 5-Me derivative (SN 7298), m. 85°, 62%, Q-B4 0.08i. 4-Chloro-5-methyl-α-(4-morpholinyl)-o-cresol (HCl salt) (SN 6796) m. 215°, 31%, Q-B4 0.05i. 4-PhC6H4OH (17 g.), 18 g. C6H4(CO)2NCH2OH, 200 cc. benzene, and 6 drops concentrated H2SO4, refluxed 2 h., evaporated to dryness, the residue in 100 cc. alc. refluxed 20 min. with 10 cc. 85% N2H4.H2O and then 1 h. with 200 cc. 3 N HCl, give 29% 4-phenyl-α-amino-o-cresol (III), light tan, m. 157-8° (HCl salt (SN 9578), m. 235°, Q-J1 1.0). Analogs of III: α-dimethylamino (SN 5017), Q-B4 0.2, Q-J1 1.0, Q-D1 0.12, Q-D2 0.25; α-diethylamino (HCl salt) (SN 7301), m. 165°, 46%, Q-B4 0.12i; α-[ethyl(2-hydroxyethyl)amino] (HCl salt) (SN 7487), m. 149°, 18%, Q-B4 0.03i; α-(1-piperidyl) (SN 7142), m. 90°, 62%, Q-B4 0.02; α-(4-morpholinyl) (SN 7143), Q-B4 0.03i; 6-hydroxy-α-diethylamino (SN 7740), m. 108°, 64%, Q-B4 0.05i, Q-J1 0.2t. 5-Phenyl-α-diethylamino-o-cresol (SN 7820) m. 78°, 76%, Q-B4 0.4, Q-J1 0.4t; 6-Ph isomer (SN 6895), Q-B4 0.2. 6-Phenyl-α-ethylamino-o-cresol (SN 9283) m. 186°, Q-B4 0.2; α-(2-hydroxyethyl)amino derivative (SN 8268), Q-B4 0.1, Q-D1 0.06, Q-D2 0.25; α-decylamino derivative (HCl salt) (SN 8298), m. 134°, 50%, Q-B4 0.13. 4-Phenyl-6-chloro-α-diethylamino-o-cresol-HCl m. 141°, 31%, Q-J1 0.17; α-1-piperidyl analog (free base) (SN 7489), m. 80°, 92%, Q-B4 0.1i. 4-Phenyl-6-bromo-α-diethylamino-o-cresol-HCl (SN 7294) m. 141°, 89%, Q-B4 0.5i. 4-Chloro-6-phenyl-α-diethylamino-o-cresol-HCl (SN 7297), m. 128°, 43%, Q-B4 0.18, Q-D1 0.5, Q-D2 1.0, Q-J1 1.0; 4-Br analog (SN 14,111), m. 146°, 70%, Q-B4 0.3. 2-Chloro-3-phenyl-α-diethylamino-o-cresol (SN 7490), m. 65°, 54%, Q-B4 0.2. 4-tert-Butyl-6-phenyl-α-dimethylamino-o-cresol-HCl (SN 7282) m. 207°, 85%, Q-B4 1.5, Q-J1 2.0; α-diethylamino analog (SN 7744), m. 173°, 83%, Q-B4 2.0, Q-D1 2.0, Q-J1 1.0i [O-Ac derivative (SN 9636), m. 201°, 67%, Q-B4 1.5; O-Me derivative (SN 10,122), m. 142°, 50%, Q-B4 0.16t; the latter was prepared from 4-tert-butyl-6-phenylanisole (b3 43-5°) through the 2-Br derivative (b2 147-8°) and its Grignard reagent]; α-ethylamino analog (SN 9557), m. 216°, 42%, Q-B4 2.5; α-(2-hydroxyethyl)-amino analog, with 2 mols. H2O (SN 9202), m. 158°, 45%, Q-B4 1.0. 4-tert-Amyl-6-phenyl-α-diethylamino-o-cresol-HCl (SN 8368), m. 168°, 80%, Q-B4 1.6, Q-D1 1.0, Q-J1 2.0. 4-(1,1,3,3-Tetramethylbutyl)-6-phenyl-α-diethylamino-o-cresol-HCl (SN 8303) m. 178%, 88%, Q-B4 0.6, Q-D1 1.0, Q-J1 0.2. 4-Phenyl-6-(3-buten-2-yl)-α-diethylamino-o-cresol-HCl (SN 8289) m. 151°, 50%, Q-D4 0.55. 4-tert-Butyl-5-phenyl-α-diethylamino-o-cresol-HCl (SN 8500) m. 190%, 83%, Q-B4 0.08. 4-Benzyl-α-diethylamino-o-cresol-HCl (SN

7499) m. 160°, 10%, Q-B4 0.13, Q-D1 0.06; 6-isomer (SN 7300) m. 149°, 48%, Q-B4 0.06, Q-D1 0.09; 4,6-dibenzyl analog (SN 14,309), m. 152°, Q-B4 0.06; 4-benzyl-6-Me analog (free base) (SN 7742), m. 106°, 59%, Q-B4 0.12t; 4-(1-methyl-1-phenylethyl) analog (SN 8049), m. 150°, 42%, Q-B4 0.05i; 4-(1-methyl-1-phenylethyl)-6-hydroxy analog (free base) (SN 8996), m. 97°, 35%, Q-B4 0.1t. 4-Substituted α-diethylamino-o-cresols: MeO (SN 7363), b3 133-5°, 52%, Q-B4 0.08i, Q-J1 0.4t; EtO (SN 7364), slightly greenish liquid, b3 144-7°, 66%, Q-B4 0.06i, Q-J1 0.4; benzyloxy (HCl salt) (SN 8371), m. 133°, 37%, Q-B4 0.04; phenoxy (HCl salt) (SN 8048), m. 130°, 39%, Q-B4 0.04, Q-J1 1.0i; 2,5-dimethyl-1-pyrryl, m. 164°, 25%, Q-B4 0.5i; 4-morpholinyl (HCl salt) (SN 8309), m. 176°, Q-B4 0.15; cyano (HCl salt) (SN 7738), m. 208°, 37%, Q-B4 0.05; the CN derivative with dry HCl in absolute EtOH gives the imido ester di-HCl salt, m. 167-9° (decomposition); shaken with EtOH-NH3, this gives 68% of the guanyl derivative (di-HCl salt) (SN 7637), m. 215°, Q-B4 0.05i. 2-Diethylaminomethyl-1-naphthol-HCl (SN 7299), m. 150°, 57%, Q-B4 0.1; 1-diethylaminomethyl-2-naphthol-HCl (SN 6806), m. 164°, 78%, Q-J1 0.1t; 7-dimethylaminomethyl-8-quinolinol-HCl, m. 186°, 74%, Q-B4 0.05i, Q-J1 0.33t; 7-(1-piperidylmethyl)-8-quinolinol, m. 194°, 52%, Q B4 0.11; 8-diethylaminomethyl-7-quinolinol, m. 220°, 37%, Q-J1 0.33t. α,α'-Bis derivs. of 4,4'-bi-o-cresols (di-HCl salts): diethylamino (SN 6894), m. 225°, 55%, Q-B4 0.17t, Q-J1 0.5i; 6,6'-dimethyl derivative (SN 7824), m. 215°, 64%, Q-B4 0.75; 6,6'-di-Pr derivative (SN 7827), m. 221°, 70%, Q-B4 1.0; 6,6'-bis(2-chloroallyl) derivative, m. 208°, 34%, Q-B4 2.5; 6,6'-bis(methallyl) derivative (SN 8379), m. 263°, 17%, Q-B4 0.11t; α,α-bis (diethylamino)-5,5'-bi-o-cresol (SN 10,271), m. 106°, 92%, Q-B4 4.0. α,α'-Bis derivs. of 6,6'-diallyl-4,4'-bi-o-cresol (di-HCl salts): dimethylamino (SN 8316), m. 241°, 47%, Q-B4 4.0; diethylamino (SN 6771), m. 209°, 67%, Q-B4 2.0, Q-J1 0.5; dipropylamino (SN 8315), m. 187°, 38%, Q-B4 1.0, Q-J1 0.5; dibutylamino (SN 8380), m. 178°, 57%, Q-B4 0.25; 1-piperidyl (SN 9558), m. 250°, 78%, Q-B4 0.5; 4-morpholinyl (SN 10,150), m. 251°, 70%, Q-B4 0.05; (2-hydroxyethylamino) (SN 9187), m. 111°, 24%, Q-B4 0.6; [bis(2-hydroxyethyl)amino] (SN 9188) m. 130°, 20%, Q-B4 0.06; O,O'-diacetyl-α,α'-bis(diethylamino) derivative (SN 9635), m. 224°, 90%, Q-B4 1.3; O,O'-dipropionyl derivative (SN 11,000), m. 185°, 30%, Q-B4 0.8. 4,4'-Oxybis(α-diethylamino-o-cresol) (SN 5918) m. 99°, 66%, Q-B4 1.0; bis-6-allyl derivative (di-HCl salt) (SN 8450), m. 240°, 47%, Q-B4 0.21. 4,4'-Isopropylidenebis(6-methyl-α-diethylamino-o-cresol)-2HCl (SN 7737) m. 210°, 48%, Q-B4 0.09; bis-6-Ph analog (free base) (SN 9186), m. 75°, 77%, Q-B4 0.5. 4,4'-(1,2-Diethyl-1,2-dihydroxy-ethylene)bis(α-diethylamino-o-cresol) (SN 7828) m. 153°, 23%, Q-B4 0.2. 4,4'-(1,2-Diethylvinylene)bis(α-diethylamino-o-cresol) (SN 7826) m. 110°, 50%, Q-B4 0.4. 4,4',4'',4'''-(Ethylenediethylidyne) tetrakis (α-diethylamino-o-cresol) (SN 8583) m. 150°, 6% Q-B4 1.4. α-Diethylamino-p-cresols: 3,6-di-Me (SN 8999), m. 104°, 20%, Q-B4 0.04i; 3-methyl-6-iso-Pr (SN 9001), m. 93°, Q-B4 0.05; 2-Ph (SN 6772), Q-B4 1.2, Q-D1 0.13, Q-J1 2.0; 2-chloro-6-Ph (HCl salt) (SN 8050), m. 162°, 80%, Q-B4 0.4, Q-D1 0.5i; 2-allyl-6-Ph (HCl salt) (SN 8388), m. 128°, 66%, Q-B4 0.4, Q-D1 0.25t; 2,6-di-Ph (HCl salt) (SN 10,210), m. 189°, 57%, Q-B4 0.12, Q-J1 1.0i. 2,4-Bis(diethylaminomethyl)-6-cyclohexylphenol-2HCl (SN 7736), m. 199°, Q-B4 0.25; 6-phenylphenol analog (2HCl) (SN 7358), m.

207°, 95%, Q-B4 1.3, Q-J1 0.5; 2,5-bis(diethylaminomethyl)hydroquin
one (SN 7356), m. 107°, 62%, Q-B4 0.23.
IT 38942-39-1, Phenol, 2-(diethylaminomethyl)-3,5-dimethyl-
(hydrochlorides)
RN 38942-39-1 CAPLUS
CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1939:29791 CAPLUS
DN 33:29791
OREF 33:4214e-g
TI Nuclear methylation of phenols. A new synthesis of intermediates in the
preparation of antisterility factors
AU Caldwell, Wm. T.; Thompson, Thomas R.
SO Journal of the American Chemical Society (1939), 61, 765-7
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 33:29791
AB One mole of 3,5-MeC6H3OH, treated with 1 mol 35% aqueous Me2NH and then at a
temperature of 25-35° with 1 mol of HCHO, gives 60 g. of
2-(dimethylaminomethyl)-3,5-dimethylphenol, m. 42-2.5°;
hydrogenation in dioxane with Cu chromite at 177 atmospheric and 165° for
4 h. gives 58.5% of 2,3,5-Me3C6H2OH. Coupling with p-NaSO3C6H4N2X,
reducing the azo dye with Na2S2O4, oxidizing the aminophenol with FeCl3
and reducing the quinone with Na2S2O4 give 27% of 2,3,5-
trimethylhydroquinone. C6H6O2 with Me2NH and HCHO gives an almost quant.
yield of 2,5-bis(dimethylaminomethyl)hydroquinone, m. 190°; reduction
gives 23% of 2,5-dimethylhydroquinone.
IT 63487-28-5P, Isopseudocumenol, α2-dimethylamino-
RL: PREP (Preparation)
(preparation of)
RN 63487-28-5 CAPLUS
CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



=>
=> FIL STNGUIDE

=>
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 233.66 | 415.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | -29.60 | -29.60

FILE 'STNGUIDE' ENTERED AT 15:25:41 ON 09 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 6, 2008 (20080606/UP).

=>
=>